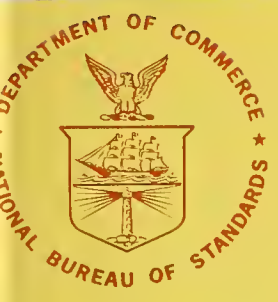

NBS MONOGRAPH 25 — SECTION 16

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

Standard X-ray Diffraction Powder Patterns

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Standard X-ray Diffraction Powder Patterns
Section 16—Data for 86 Substances

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Boris Paretzkin, and Johan H. de Groot

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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Previous work has been published as a book entitled *Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards* (1976) (JCPDS--International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081). The volume is sold with an accompanying search manual, and contains 949 card images of patterns of experimental data, published originally as Circular 539 (vols. 1-10) and Monograph 25, Sections 1-12, and most of Section 13.

Individual copies of the Circular and Monograph are still available and may be obtained from the National Technical Information Service, 5285 Port Royal Road, Springfield, VA 22161. If a publication listed below is identified with a number, it must be used in ordering. All are available in hardcopy or microfiche; the price is not fixed and will be furnished on request.

NBS Publication	Number
Circular 539, Volume 1	PB 178 902
Volume 2	PB 178 903
Volume 3	PB 178 904
Volume 4	PB 178 905
Volume 5	PB 178 906
Volume 6	PB 178 907
Volume 7	PB 178 908
Volume 8	PB 178 909
Volume 9	PB 178 910
Volume 10	PB 178 911

NBS Publication	Number
Monograph 25, Section 1	PB 178 429
Section 2	PB 178 430
Section 3	PB 178 431
Section 4	
Section 5	
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Section 7	
Section 8	PB 194 872
Section 9	COM 72-50002
Section 10	COM 72-51079
Section 11	COM 74-50183
Section 12	COM 75-50162
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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 16. --- Data for 86 Substances

by

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Boris Paretzkin, and Johan H. de Groot
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and

Camden R. Hubbard and Simon J. Carmel
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Standard x-ray diffraction patterns are presented for 86 substances. Fifty-eight of these patterns represent experimental data and 28 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

Key words: Crystal structure; integrated intensities; lattice constants; peak intensities; powder patterns; reference intensities; standard; x-ray diffraction.

INTRODUCTION

The Powder Diffraction File is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the [1] JCPDS--International Centre for Diffraction Data, the File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the JCPDS, the program at the National Bureau of Standards contributes new data to this File. Our work also aids in the evaluation and revision of published x-ray data and in the development of diffraction techniques. This report presents information for 86 compounds (58 experimental and 28 calculated patterns), and is the twenty-sixth of the series of "Standard X-ray Diffraction Powder Patterns "[2].

EXPERIMENTAL POWDER PATTERNS

CAS registry number. The Chemical Abstracts Service Registry Number is included, when available, to help identify the sample. This number forms the basis for computer aided searching of Chemical Abstracts.

Sample. The samples used to make NBS patterns were obtained from a variety of sources or were prepared in small quantities in our laboratory. Appropriate annealing or recrystallization of the samples improved the quality of most of the patterns. A check of phase purity was provided by indexing the x-ray pattern.

Optical data. When reported, optical measurements were made by grain immersion methods, in white light, using oils standardized in sodium light, in the refractive index range 1.49 to 2.1 [Hartshorne and Stuart, 1970].

The names of the sample colors were selected from the ISCC-NBS Centroid Color Charts [1965].

Interplanar spacings. For spacing determinations, a shallow holder was packed with a sample mixed with an internal standard. Choice of the standard was determined by the need for low angle and unobstructed reflections. The amount of standard was estimated so that the intensity of its strongest peak would be about equal to the intensity of the strongest peak of the sample.

To avoid errors associated with aberrations at the very top of the peaks, the readings of 2θ were taken at positions about 20% of the way down from the top, and in the center of the peak width. The $K\alpha_2$ peaks were occasionally read to assist in establishing a $K\alpha_1$ peak position, but $K\alpha_2$ peaks were not reported.

At low angles, $K\alpha_1$ and $K\alpha_2$ peaks were unresolved for both the sample and the internal standard. The internal standard corrections were established from the theoretical values for $K\alpha_1$ and were applied to the unresolved low angle peaks, as well as to the resolved $K\alpha$, peaks in the higher angle regions. If the internal standard correction varied along the length of the pattern, linear interpolations were used.

[1] JCPDS--International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA. 19081. This Pennsylvania non-profit corporation functions in cooperation with the American Ceramic Society, the American Crystallographic Association, the American Society for Testing and Materials, The Clay Minerals Society, The Institute of Physics, the Mineralogical Association of Canada, the Mineralogical Society of America, The Mineralogical Society of Great Britain and Ireland, the National Association of Corrosion Engineers, and the Société Française de Minéralogie et de Cristallographie.

[2] See previous page for other published volumes.

The internal standards used were of high purity (99.99%). The lattice constants used for them at 25 °C are given in Table 1; the 2θ angles were computed using cell dimensions uncorrected for index of refraction.

Table 1

Calculated 2θ Angles, $CuK\alpha_1$ λ = 1.540598Å

hkℓ	W a=3.16524Å ±.00004	Ag a=4.08651Å ±.00002	Si a=5.43088Å ±.00004
110	40.262		
111		38.112	28.443
200	58.251	44.295	
211	73.184		
220	86.996	64.437	47.303
310	100.632		
311		77.390	56.123
222	114.923	81.533	
321	131.171		
400	153.535	97.875	69.131
331		110.499	76.377
420		114.914	
422		134.871	88.032
511/333		156.737	94.954
440			106.710
531			114.094
620			127.547
533			136.897
444			158.638

The new internal standard Si powder is available as Standard Reference Material 640 [1974]. The lattice constant for the Si was refined from multiple powder data measurements made with tungsten as an internal standard [Swanson et al., 1966]. Cell parameter data were also collected for single crystal from the boules ground to prepare the powder. The lattice parameters from the two methods agreed within 3 parts in 10^5 [Hubbard et al. 1975]. D-spacing results using SRM 640 will be in agreement with patterns recorded in this series of monographs since 1966.

All of our spacing measurements were recorded at 25 ± 1 °C on a diffractometer equipped with a focusing graphite or lithium fluoride crystal monochromator located between the sample and the scintillation counter. Pulse height discrimination was used as well. All measurements were performed using copper radiation: λ($CuK\alpha_1$, peak)=1.540598Å [Deslattes and Henins, 1973].

Structure, lattice constants. The space groups were listed with short Hermann-Mauguin symbols as well as the space group numbers given in the *International Tables for X-ray Crystallography, Vol. I* [1952].

Orthorhombic cell dimensions were arranged according to the Dana convention b>a>c [Palache et al., 1944]. Monoclinic and triclinic lattice constants were transformed if necessary in order to follow the convention of *Crystal Data* [1973].

A computer program [Evans et al., 1963] assigned hkℓ's and refined the lattice constants. Cell refinement was based only upon $2\theta_{obs}$ values which could be indexed without ambiguity. The program minimized the value $\Sigma(\theta_{obs}-\theta_{calc})^2$. The estimated standard deviations (e.s.d.'s) of the reciprocal cell parameters were determined from the inverse matrix of the normal equations. The program calculated the e.s.d.'s of the direct cell constants by the method of propagation of errors. Since 1973, the e.s.d.'s derived by the computer program have been increased by 50% in order to reflect more truly the uncertainty in the lattice constants. A similar increase should also be applied to all lattice constants in earlier publications of this series. The e.s.d.'s in the least significant figures are given in parentheses following the lattice constants.

In indexing cubic patterns, multiple hkℓ's were not utilized in the refinement or reported. Instead, the single appropriate index having the largest h was listed. The number of significant figures reported for d-values varied with the symmetry and crystallinity of each sample.

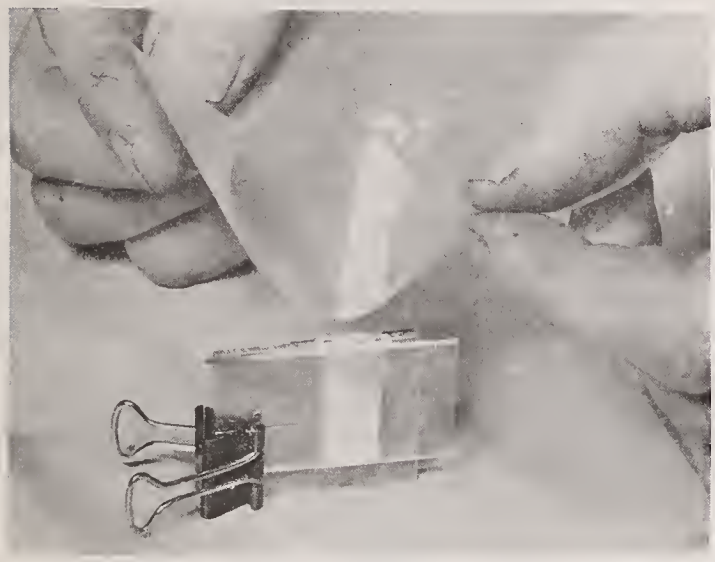
Densities. These were calculated from the specified lattice constants, the Avogadro number 6.0220943×10^{23} [Deslattes et al., 1974] and atomic weights published by the International Union of Pure and Applied Chemistry [1972].

Figure of merit. Several figures of merit ratings are available for assessing indexed powder data. M_{20} [de Wolff, 1968] is a criterion for the reliability of the unit cell and indexing. A value of $M_{20} > 10$ will guarantee the essential correctness of the indexing provided there are not more than 2 spurious lines ($X_{20} \leq 2$) [de Wolff, 1968]. All patterns reported in this publication have M_{20} between 20 and 233, and $X_{20} = 0$ unless noted otherwise. M_{20} was specified for any pattern indexed with a cell derived only through computer indexing from powder data, without further confirmation.

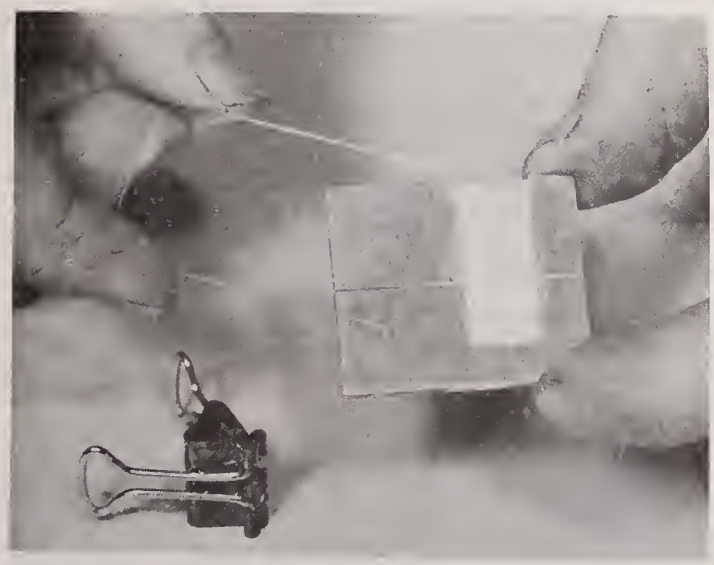
The accuracy and completeness of measured interplanar spacings is conveniently reported as F_N [Smith and Snyder, 1979]. The format used in this publication was F_N = overall value ($|\overline{\Delta 2\theta}|$, N_{poss}), where N, the number of observed reflections was chosen as 30 or the maximum number of lines of the pattern, if the entire pattern had fewer than 30 lines. The "overall value" was the figure of merit, F_N, as defined by Smith and Snyder [1979], and $|\overline{\Delta 2\theta}|$ was the average absolute magnitude of discrepancy between observed and calculated 2θ values for the N lines. N_{poss} was the number of unique and resolvable diffraction lines allowed in the space group, up to the N^{th} observed and indexed line. In this publication, the value of F_N ranged from 31 to 118, with an average value of 61 for the 58 patterns from experimental data.

Intensity measurements. It was found that samples which gave satisfactory intensity patterns usually had an average particle size smaller than 10 μm, as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed,

a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Figure 1), and the powdered sample was allowed to drift into the end opening while the holder was held in a vertical position.



With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (see Figure 2). If the sample powder did not flow readily, or was prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the strongest line. Any intensity larger than 20 was rounded to the nearer multiple of 5. At least 3 patterns for intensity measurements were prepared for each sample to check reproducibility.



Reference Intensity Ratio, $I/I_{corundum}$. The reference intensity ratio, I/I_c, has been defined as the direct ratio of the intensity of the strongest reflection of a sample, to the intensity of the reflection 113 (hexagonal) of corundum (α-Al_2O_3) [Visser and de Wolff, 1964]. In this publication, the ratios I/I_c were tabulated for copper K$\bar{\alpha}$ radiation, for a 1:1 mixture by weight of the sample and corundum. Occasionally I/I_c was not determined because it was not feasible.

A procedure has been adopted, to achieve greater statistical accuracy [Hubbard and Smith, 1977]. For any weight fractions of sample and corundum, x_s and x_c ($x_s = 1-x_c$), the intensities for reflection $\underline{h}$ of the sample and $\underline{k}$ of corundum were measured for several combinations of $\underline{h}$ and $\underline{k}$ usually within the same region of 2θ, to provide indications of possible preferred orientation, extinction, or other systematic errors. The reference intensity ratio is then given by

$$\frac{I(\underline{h}_0)}{I_c(113)} = \frac{x_c}{x_s} \cdot \frac{I_c^{rel}(\underline{k})}{I^{rel}(\underline{h})} \cdot \frac{I(\underline{h})}{I(\underline{k})}$$

and $(\underline{h}_0)$ indicates specifically which reflection was chosen for tabulation purposes. For each of our patterns, the reflection $(\underline{h}_0)$ will be the one with I=100 since only copper radiation was used. Typically, at least 3 sets of reflections and 2 mountings of the mixture were used to obtain 6 or more values for the reference intensity ratio, I/I_c. These values yield the tabulated average $\langle I/I_c \rangle$. From these data, the estimated deviation, Δ, was obtained from

$$\Delta = \frac{\sum_{i=1}^{n} \left| (I/I_c)_i - \langle I/I_c \rangle \right|}{n}$$

where n is the number of measurements of the reference intensity ratio. The estimated deviation in the least significant figures is given in parentheses.

Format of tables. The printing of the data has been computerized. Superimposed reflections were treated in one of two ways. If a d-spacing had only two possible indices, an M was added to the d-spacing which was repeated on the next line, but with the second index. However, if there were more than two possible indices, a + sign was used in like manner. In both cases, the composite intensity was printed only once and aligned with the first reflection. The symbol "1L" in the intensity column was used to indicate "less than 1."

CALCULATED POWDER PATTERNS

Since some substances of interest are not readily available for experimental work, powder patterns were calculated from published crystal structure data. The FORTRAN program used for the computations was developed by Clark et al. [1973] and modified at NBS.

Lattice parameters. Before the computations of the patterns, any necessary changes were made

in the lattice constants in order to make them consistent with the revised value of $\lambda(CuK\alpha_1)$= 1.540598Å [Deslattes and Henins, 1973]. Both the altered and the original published values are given. A lattice constant arrangement which follows the convention of *Crystal Data* has been referred to as the "CD cell." In several of the calculated patterns, the literature lattice constants, the atom positions, and hence the final patterns were not given in the CD arrangement. For cross-reference purposes, the CD cell was calculated separately and included in the text.

Scattering factors. Whenever possible, the same scattering factors were used which the author of the reference article specified. Otherwise, the factors were taken directly from the *International Tables for X-ray Crystallography, Vol. III,* [1962]. The factors were corrected for dispersion if the author had done so.

Thermal parameters. The computer program used thermal parameter data of only two forms, the isotropic B's ($Å^2$) or the anisotropic β_{ij}'s in the following expressions:

$$e^{(-B \sin^2\theta)/\lambda^2}$$

or

$$e^{-(h^2\beta_{11}+k^2\beta_{22}+\ell^2\beta_{33}+2hk\beta_{12}+2h\ell\beta_{13}+2k\ell\beta_{23})}.$$

Other thermal parameters (e.g. U_{ij}) were converted to one of these two forms. The isotropic parameters were used directly, if given by the structure reference. In a few of our patterns, anisotropic parameters were also used directly as given by the structure reference; in other work, instead of using given anisotropic parameters, approximately equivalent isotropic values were substituted as defined by:

$$B = 4\left[\frac{\beta_{11}\beta_{22}\beta_{33}}{a^{*2}\ b^{*2}\ c^{*2}}\right]^{\frac{1}{3}}$$

Structural information. The atom positions used in these calculated patterns varied somewhat in the degree of reliability. In our text, when the expression "the structure was determined by..." was used, the atomic parameters in the reference cited had been calculated from refinement of single crystal data. Otherwise, the atomic positions had been derived by analogy with similar compounds whose structure was known. In cases where isostructural relationships were used, the atoms were in fixed special positions or the ionic radii were closely related to the corresponding radii of the atoms in the known structure.

Integrated intensities. The theoretical integrated intensity of reflection i on the "absolute-relative" scale is I_i^{abs}/K, as defined by Hubbard et al. [1976] in the equation

$$\frac{I_i^{abs}}{K} = \frac{M_i Lp_i |F_i T_i|^2}{2\mu V^2}$$

where:

F is the structure factor
T is the thermal correction

$Lp = \frac{1+\cos^2 2\theta}{\sin^2\theta\cos\theta}$ is the Lorentz-polarization term

M is the multiplicity for the reflection i
μ is the linear absorption coefficient
V is the volume of the unit cell.

When the largest integrated intensity was assigned a relative value of 100 and all other reflections were scaled relative to it, the intensities were placed on the relative intensity scale (I^{rel}). Reflections with I^{rel} less than 0.7 were omitted. Relative intensities were rounded to the nearest integer value before being listed, except that for phases whose structures were postulated or were based on analogy, any intensity above 20 was rounded further, to the nearer multiple of 5.

Scale factor (integrated intensities). The scale factor, γ, was defined to convert the tabulated I^{rel} to the "absolute-relative" scale [Hubbard et al., 1976]. That is:

$$\gamma = \frac{M'Lp'|F'T'|^2}{200\mu V^2}$$

and

$$\frac{I^{abs}}{K} = \gamma I^{rel}$$

The primes denoted the values for the largest integrated intensity. In earlier Monographs (1969-1975), a different scale factor, k_{NBS}, was reported which is related to γ:

$$\frac{\gamma}{k_{NBS}} = \frac{1}{2\mu V^2}$$

From γ, the theoretical value of the Reference Intensity Ratio, I/I_c, was calculated:

$$I/I_c = \frac{\mu\gamma\rho_c}{\mu_c\gamma_c\rho}$$

where ρ is the density and the subscript c represents corundum (α-Al_2O_3).

For refined structures, the value of I/I_c was given. For those phases whose structures were postulated or were based only on analogy to other powder patterns, I/I_c was not included.

I/I_c and γ are each based on the single strongest reflection, not on the overlapping sum of superimposed reflections.

Peak heights. The purpose of calculating peak height intensity was to provide a tabulated pattern similar to what might be obtained from experimental diffractometer measurements. For each predicted reflection, Cauchy profiles centered at both the α_1 and the α_2 peak positions were calculated and summed, forming a simulated powder pattern. The full width at half-maximum (FWHM)

was allowed to vary to represent the changing FWHM as a function of 2θ. [The values of the FWHM vs 2θ are given in Table 2.]. The resultant simulated powder pattern was then analyzed for peaks. In the regions of the predicted reflections several reflections could have identical or similar 2θ angles and produce only one composite peak in the simulated pattern. The 2θ angle of the composite peak was assigned the hkℓ of the reflection having the greatest contribution to the peak height intensity. If any other peak contributed more than 10% of the intensity toward the composite peak height intensity, a plus sign(+) was appended to the hkℓ.

Peaks due solely to α_2 lines were omitted. If a composite peak was formed by the overlap of an α_1 peak of reflection j with the α_2 peak of reflection i, the reflection j was listed separately only if it contributed a significant intensity (>10%) at the composite peak location.

The peak search routine located peaks only at 2θ angles which were a multiple of 0.02°.

Table 2

2θ CuKα_1	FWHM	2θ CuKα_1	FWHM
0°	0.12°	140	0.230
20	.12	145	.255
40	.12	150	.285
60	.125	155	.315
80	.130	160	.360
100	.135	162.5	.410
120	.155	165	.500
130	.185		

UNITS

In this publication the Ångström unit (1Å= 100pm) was selected for presentation of the d-spacings and lattice parameters to maintain consistency with (a) the earlier publications of Standard X-ray Diffraction Powder Patterns (Circular 539 volumes 1-10 and Monograph 25 sections 1-15), (b) the publications of the International Union of Crystallography: Acta Crystallographica and the Journal of Applied Crystallography, and (c) the continuing publication of cards and search manuals of the Powder Diffraction File (now consisting of nearly 30,000 entries). The PDF search manuals are based on the d-spacings in Å of the three strongest lines. Consistent with the choice of the Å unit for length, the volume of the unit cell is expressed in $Å^3$ (=1 x 10^{-30} m^3). Other reported parameters and their units are density in g/cm^3 (1 gm/cm^3 = 10^{-3} kg/m^3) and the linear absorption coefficient in cm^{-1}.

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ISCC-NBS Centroid Color Charts, SRM 2106, or Color Kit, SRM 2107 which contains both SRM 2106 and *Color,* an NBS Special Publication #SP 440. These can be obtained from the National Bureau of Standards, Office of Standard Reference Materials, Washington, D.C. 20234. Current prices will be quoted on request.

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Acetanilide, C_8H_9NO

CAS registry no.
103-84-4

Sample
The sample is Standard Reference Material 141c of the National Bureau of Standards, obtained from J. T. Baker Co., Phillipsburg, NJ. It is used for checking microchemical procedures for the determination of carbon, hydrogen and nitrogen in organic matter.

Color
Colorless

Structure
Orthorhombic, Pcab (61), Z = 8. The structure was determined by Brown and Corbridge [1954] and refined by Brown [1966].

Lattice constants of this sample
a = 9.494(3) Å
b = 19.645(4)
c = 7.995(2)

a/b = 0.4833
c/b = 0.4070

Volume
1491. Å^3

Density
(calculated) 1.204 g/cm^3

Figure of merit
F_{30} = 56.3 (0.013,40)

Reference intensity
$I/I_{corundum}$ = 0.63(4)

Additional patterns
1. PDF card 18-1501 [Billig, B. and Greenberg, B., Polytechnic Institute of Brooklyn, 1965]
2. Morris et al. [1977]

References

Brown, C. J. (1966). Acta Crystallogr. 21, 442.

Brown, C. J. and Corbridge, D. E. C. (1954). Acta Crystallogr. 7, 711.

Morris, M. C., McMurdie, H. F., Evans, E. H., Paretzkin, B., de Groot, J. H., Newberry, R., Hubbard, C. R., and Carmel, S. J. (1977). Nat. Bur. Std. U.S. Monogr. 25, Sec. 14, 38.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
9.81	90	0 2 0	9.01
6.82	30	1 2 0	12.97
5.84	65	1 1 1	15.17
5.193	30	1 2 1	17.06
4.913	5	0 4 0	18.04
4.749	6	2 0 0	18.67
4.469	30	1 3 1	19.85
4.360	30	1 4 0	20.35
4.273	8	2 2 0	20.77
4.081	45	2 0 1	21.76
3.994M	60	0 0 2	22.24
3.994M		2 1 1	22.24
3.917	55	0 1 2	22.68
3.826	19	1 4 1	23.23
3.768	40	2 2 1	23.59
3.700	100	0 2 2	24.03
3.620	30	1 1 2	24.57
3.448	55	1 2 2	25.82
3.411M	10	2 4 0	26.10
3.411M		0 3 2	26.10
3.305	7	1 5 1	26.96
3.210	20	1 3 2	27.77
3.097M	9	0 4 2	28.80
3.097M		1 6 0	28.80
2.773	5	2 3 2	32.26
2.694	5	2 6 0	33.23
2.658	2	3 4 0	33.69
2.597	8	2 4 2	34.51
2.549	7	1 7 1	35.18
2.543	8	1 1 3	35.27
2.535	7	0 6 2	35.38
2.482	4	1 2 3	36.16
2.455	2	0 8 0	36.58
2.414	2	2 5 2	37.21
2.378	6	1 8 0	37.80
2.355	2	3 5 1	38.18
2.308M	6	2 1 3	39.00
2.308M		4 2 0	39.00
2.297	7	0 7 2	39.18
2.277+	6	3 6 0	39.55
2.277+		4 0 1	39.55

d(A)	I	hkℓ	2θ(°)
2.214	2	3 4 2	40.73
2.191	5	2 3 3	41.17
2.148M	2	4 3 1	42.02
2.148M		1 5 3	42.02
2.099	2	3 5 2	43.07
2.067	3	2 7 2	43.76
2.056	4	1 9 1	44.00
2.030M	2	3 7 1	44.60
2.030M		4 1 2	44.60
2.027	4	3 1 3	44.67
1.969	3	4 5 1	46.05
1.965	2	0 10 0	46.17
1.947M	5	3 3 3	46.62
1.947M		1 1 4	46.62
1.923M	5	4 6 0	47.23
1.923M		1 10 0	47.23
1.919	5	1 2 4	47.32
1.895M	4	2 6 3	47.98
1.895M		1 7 3	47.98
1.885M	5	3 8 1	48.24
1.885M		4 4 2	48.24
1.879	6	1 9 2	48.41
1.870	4	1 10 1	48.65

Ammonium Hydrogen Arsenate, $NH_4H_2AsO_4$

Sample
The sample was obtained from Alfa Products, Danvers, MA.

Color
Colorless

Structure
Tetragonal, $I\bar{4}2d$ (122), Z = 4, isostructural with KH_2PO_4. The structure was determined by Delain [1958] and refined by Khan and Bauer [1973].

Lattice constants of this sample
a = 7.6978(6) Å
c = 7.7193(7)

c/a = 1.0028

Volume
457.41 Å^3

Density
(calculated) 2.308 g/cm^3

Figure of merit
F_{30} = 76.2(0.012,32)

Reference intensity
$I/I_{corundum}$ = 4.3(2)

Additional pattern
1. PDF card 1-775 [Hanawalt et al., 1938]

References
Delain, C. (1958). C. R. Acad. Sci. Ser. C 247, 1451.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Khan, A. A. and Baur, W. H. (1973). Acta Crystallogr. B29, 2721.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
5.450	80	1 0 1	16.25
3.847	65	2 0 0	23.10
3.143	100	2 1 1	28.37
2.725	15	2 0 2	32.84
2.719	20	2 2 0	32.91
2.438	4	1 0 3	36.83
2.433M	4	3 1 0	36.92
2.433M		3 0 1	36.92
2.058M	45	3 2 1	43.96
2.058M		3 1 2	43.96
1.929	1	0 0 4	47.07
1.924	3	4 0 0	47.20
1.8166	9	3 0 3	50.18
1.8142	9	4 1 1	50.25
1.7252	10	2 0 4	53.04
1.7218M	12	4 0 2	53.15
1.7218M		4 2 0	53.15
1.6427M	12	3 2 3	55.93
1.6427M		3 3 2	55.93
1.5738	6	2 2 4	58.61
1.5106M	11	4 1 3	61.32
1.5106M		5 0 1	61.32
1.4058M	10	5 1 2	66.45
1.4058M		5 2 1	66.45
1.3629	6	4 0 4	68.83
1.3607	4	4 4 0	68.96
1.3231	2	3 0 5	71.21
1.3213	2	4 3 3	71.32
1.2847	5	4 2 4	73.68
1.2829	3	6 0 0	73.80
1.2519	4	1 1 6	75.95
1.2489M	7	6 1 1	76.16
1.2489M		5 3 2	76.16
1.2175M	4	6 0 2	78.50
1.2175M		6 2 0	78.50
1.1900	2	4 1 5	80.68
1.1877	1	5 4 1	80.87
1.1376	2	3 1 6	85.24
1.1352M	3	6 3 1	85.46
1.1352M		6 1 3	85.46
1.1120	1L	4 4 4	87.69
1.0917	1L	1 0 7	89.76
1.0886M	3	7 1 0	90.08
1.0886M		7 0 1	90.08
1.0675	2	6 4 0	92.37
1.0501	2	2 1 7	94.37
1.0476M	5	7 2 1	94.66
1.0476M		5 5 2	94.66
1.0296	2	6 2 4	96.86
1.0113	1L	7 0 3	99.23

Ammonium Titanium Fluoride, $(NH_4)_2TiF_6$

CAS registry no.
16962-40-7

Sample
The sample was donated by Harshaw Chemical Co., Cleveland, OH.

Color
Colorless

Structure
Hexagonal, $P\bar{3}ml$ (164), Z = 1, isostructural with K_2GeF_6 [Cox and Sharpe, 1953].

Lattice constants of this sample
a = 5.9456(4) Å
c = 4.8053(5)
c/a = 0.8082

Volume
147.11 $Å^3$

Density
(calculated) 2.235 g/cm^3

Figure of merit
F_{24} = 98.9 (0.010,25)

Reference intensity
$I/I_{corundum}$ = 1.38(7)

Reference
Cox, B. and Sharpe, A. G.(1953). J. Chem. Soc. 1953, 1783.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C Internal standard Ag, a = 4.08651 Å					
d(Å)	I	h	k	ℓ	2θ(°)
5.151	100	1	0	0	17.20
4.808	25	0	0	1	18.44
3.513	80	1	0	1	25.33
2.972	14	1	1	0	30.04
2.574	4	2	0	0	34.82
2.527	6	1	1	1	35.49
2.402	7	0	0	2	37.41
2.269	85	2	0	1	39.69
2.1767	7	1	0	2	41.45
1.9451	2	2	1	0	46.66
1.8686	10	1	1	2	48.69
1.8035	14	2	1	1	50.57
1.7569	20	2	0	2	52.01
1.7165	1	3	0	0	53.33
1.6167	4	3	0	1	56.91
1.5293	2	1	0	3	60.49
1.5130	9	2	1	2	61.21
1.4863	10	2	2	0	62.43
1.4284	3	3	1	0	65.27
1.4197	4	2	2	1	65.72
1.4102	5	1	1	3	66.22
1.3964	3	3	0	2	66.96
1.3690	5	3	1	1	68.48
1.3601	5	2	0	3	68.99

p-Anisic Acid, $C_8H_8O_3$

Synonym
1. 4-Methoxybenzoic Acid

CAS registry no.
100-09-4

Sample
The sample was NBS Standard Reference Material 142, a microanalytical standard for the methoxyl radical.

Color
Colorless

Structure
Monoclinic, $P2_1/a$ (14), Z = 4 [Rokade et al., 1942]. A qualitative structure was done by Richards [1956].

Lattice constants of this sample
a = 16.899(4) Å
b = 10.971(3)
c = 3.976(2)
β = 95.41(2)°

a/b = 1.5403
c/b = 0.3624

Volume
733.86 Å^3

Density
(calculated) 1.377 g/cm^3

Figure of merit
F_{30} = 40.4(0.016,48)

Additional pattern
1. PDF card 11-765 [Institute of Physics, University College, Cardiff, Wales, 1961]

References

Richards, J. P. G. (1956). Res. Appl. Ind. 9, S44.
Rokade, R. K., Khabaria, R. H., and Kapadia, M. R. (1942). J. Univ. Bombay 11, 37.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
9.18	6	1 1 0	9.63
8.40	5	2 0 0	10.52
6.69	9	2 1 0	13.23
5.48	95	0 2 0	16.15
5.221	25	1 2 0	16.97
4.598	3	2 2 0	19.29
3.924M	14	4 1 0	22.64
3.924M		3 2 0	22.64
3.720M	12	0 1 1	23.90
3.720M		-2 0 1	23.90
3.569M	13	1 3 0	24.93
3.569M		1 1 1	24.93
3.523	100	-2 1 1	25.26
3.340	6	4 2 0	26.67
3.298	5	2 1 1	27.01
3.213M	3	5 1 0	27.74
3.213M		0 2 1	27.74
3.077	30	-2 2 1	29.00
2.983	2	3 1 1	29.93
2.921	3	-4 1 1	30.58
2.880	2	-3 2 1	31.03
2.869	2	5 2 0	31.15
2.802	3	6 0 0	31.91
2.754	3	4 0 1	32.48
2.745	2	0 4 0	32.60
2.707	1	1 4 0	33.06
2.673	5	4 1 1	33.50
2.626	2	1 3 1	34.12
2.606M	3	2 4 0	34.38
2.606M		-2 3 1	34.38
2.512	3	2 3 1	35.72
2.496	3	6 2 0	35.95
2.474	4	5 3 0	36.28
2.465M	5	3 4 0	36.42
2.465M		4 2 1	36.42
2.416	1	-5 2 1	37.19
2.398	1	-6 0 1	37.47
2.392	1	5 1 1	37.57
2.365	1	3 3 1	38.01
2.348	3	7 1 0	38.31
2.297	2	4 4 0	39.19
2.250	2	-1 4 1	40.05
2.240	1	5 2 1	40.22
2.227	1	6 3 0	40.48
2.207	1	-2 4 1	40.86

p-Anisic Acid, $C_8H_8O_3$ - (continued)

d(Å)	I	hkℓ	2θ(°)
2.200M	1	7 2 0	40.99
2.200M		4 3 1	40.99
2.196	2	-6 2 1	41.06
2.176	1	1 5 0	41.47
2.169	3	-5 3 1	41.61
2.149M	4	6 1 1	42.01
2.149M		2 4 1	42.01
2.125M	2	5 4 0	42.51
2.125M		2 5 0	42.51
2.102	3	8 0 0	43.00
2.065	3	8 1 0	43.81
2.043	2	3 5 0	44.31
2.037M	2	5 3 1	44.45
2.037M		6 2 1	44.45
2.008	1	7 3 0	45.11
1.999	1	-7 2 1	45.32
1.969	1	-2 0 2	46.05
1.964	2	8 2 0	46.19
1.961	2	6 4 0	46.25
1.945M	3	4 5 0	46.67
1.945M		4 4 1	46.67

Antimonic Acid, $H_{14}Sb_{14}O_{21}(OH)_{42}$

Sample
The sample was prepared by dissolving Sb metal in warm HCl and HNO_3 (both concentrated). With constant stirring, the solution was poured into water at 80 °C. Stirring was continued overnight at 70 °C. The crystals formed were filtered off and dried in air at room temperature. The water content varies somewhat but causes little change in the x-ray pattern [Abe and Ito, 1968; Stewart et al., 1972]. The material is often referred to as "$Sb_2O_5 \cdot 4H_2O$."

Color
Colorless

Structure
Cubic, Fd3m (227), Z = 1. The structure was determined by Baetsle and Huys [1968]. Dehydrated phases have powder patterns similar to that of $H_{14}Sb_{14}O_{21}(OH)_{42}$ in d-spacings and cell size, but are quite distinct in relative intensities [Stewart et al., 1972].

Lattice constant of this sample
a = 10.3553(7) Å

Volume
1110.4 Å^3

Density
(calculated) 4.140 g/cm^3

Figure of merit
F_{20} = 54.9(0.012,31)

Reference intensity
$I/I_{corundum}$ = 3.49(10)

Additional patterns
1. PDF card 20-111, labeled $Sb_2O_5 \cdot 4H_2O$ [Baetsle and Huys, 1968]
2. PDF card 21-803, labeled $Sb_2O_5 \cdot 4H_2O$ [Abe and Ito, 1968]
3. Natta and Baccaredda [1936]
4. Hanawalt et al. [1938]

References

Abe, M. and Ito, T. (1968). Bull. Chem. Soc. Jap. 41, 333.
Baetsle, L. H. and Huys, D. (1968). J. Inorg. Nucl. Chem. 30, 639.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Ed. 10, 457.
Natta, G. and Baccaredda, M. (1936). Gazz. Chim. Ital. 66, 308.
Stewart, D. J., Knop, O., Ayasse, C., and Woodhams, F. W. D. (1972). Can. J. Chem. 50, 690.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
5.993	100	1 1 1	14.77
3.123	70	3 1 1	28.56
2.989	90	2 2 2	29.87
2.590	20	4 0 0	34.61
2.376	10	3 3 1	37.83
2.115	3	4 2 2	42.72
1.9928	17	5 1 1	45.48
1.8302	35	4 4 0	49.78
1.7503	20	5 3 1	52.22
1.5789	10	5 3 3	58.40
1.5607	25	6 2 2	59.15
1.4950	6	4 4 4	62.03
1.4506	12	7 1 1	64.15
1.3479	10	7 3 1	69.71
1.1877	7	6 6 2	80.87
1.1576	6	8 4 0	83.43
1.1366	4	9 1 1	85.33
1.0856	2	9 3 1	90.40
1.0569	3	8 4 4	93.58
1.0408	4	7 7 1	95.48

Antimony Oxide, Sb_6O_{13}

CAS registry no.
12165-47-8

Sample
The sample was prepared by heating antimonic acid ($H_{14}Sb_{14}O_{21}(OH)_{42}$) at 780 °C for 30 minutes.

Color
Colorless

Structure
Cubic, Fd3m (227), Z = 4. Defect pyrochlore structure [Stewart et al., 1972]. This material has been reported as Sb_2O_5 [Swanson et al., 1960] and as $Sb_3O_6(OH)$ (stibiconite) [Dihlström and Westgren, 1937]. The composition of the mineral stibiconite is uncertain [Vitaliano and Mason, 1952].

Lattice constant of this sample
a = 10.3060(2) Å

Volume
1094.6 Å^3

Density
(calculated) 5.696 g/cm^3

Figure of merit
F_{30} = 71.6(0.010,40)

Additional patterns
1. PDF card 11-690 [Swanson et al., 1960] called Sb_2O_5
2. PDF card 16-938 [Dihlström and Westgren, 1937] called $Sb_3O_6(OH)$
3. PDF card 21-51 [Ito et al., Tokyo Institute of Technology, 1966].
4. Natta and Baccaredda [1936]
5. Stewart et al. [1972]

References

Dihlström, K. and Westgren, A. (1937). Z. Anorg. Allg. Chem. 235, 153.
Natta, G. and Baccaredda, M. (1936). Gazz. Chim. Ital. 66, 308.
Stewart, D. J., Krop, O., Ayasse, C., and Woodhams, F. W. D. (1972). Can. J. Chem. 50, 690.
Swanson, H. E., Cook, M. I., Evans, E. H., and de Groot, J. H. (1960). Nat. Bur. Stand. U.S. Circ. 539, 10, 10.
Vitaliano, C. J. and Mason, B. (1952). Amer. Mineral. 52, 982.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

c(Å)	I	hkℓ	2θ(°)
5.949	25	1 1 1	14.88
3.108	20	3 1 1	28.70
2.976	100	2 2 2	30.00
2.577	30	4 0 0	34.78
2.365	4	3 3 1	38.02
2.1022	2	4 2 2	42.99
1.9833	6	5 1 1	45.71
1.8213	25	4 4 0	50.04
1.7416	8	5 3 1	52.50
1.6293	1L	6 2 0	56.43
1.5716	2	5 3 3	58.70
1.5535	30	6 2 2	59.45
1.4876	9	4 4 4	62.37
1.4432	8	5 5 1	64.52
1.3416	6	7 3 1	70.08
1.2885	4	8 0 0	73.43
1.2592	1	7 3 3	75.43
1.1902	1	7 5 1	80.66
1.1822	8	6 6 2	81.32
1.1522	8	8 4 0	83.91
1.1313	4	9 1 1	85.83
1.0805	3	9 3 1	90.94
1.0519	6	8 4 4	94.16
1.0360	3	7 7 1	96.07
.9965	2	9 5 1	101.25
.9918	4	10 2 2	101.92
.9611	3	9 5 3	106.54
.9291	1	11 1 1	112.00
.9109	2	8 8 0	115.49
.9004	6	9 7 1	117.63
.8742	6	9 7 3	123.57
.8710	8	10 6 2	124.35
.8588	6	12 0 0	127.51
.8500	3	11 5 1	129.98
.8277	2	11 5 3	137.06
.8148	5	12 4 0	141.96
.8072	2	9 9 1	145.20

Antimony Tin, SbSn

CAS registry no.
28980-49-6

Sample
The sample was made by melting Sn and Sb together above 1100 °C in air. It was then quenched by pouring out onto a slab, and ground. This phase has a homogeneity range of 45-55 percent Sb [Hägg and Hybinette, 1935].

Color
Black

Structure
Hexagonal, R**, Z = 3. This phase was studied by Hägg and Hybinette [1935]. These authors reported a rhombohedral cell with both a and c doubled. No lines were found in the authors' pattern or the NBS pattern that required the larger cell. This phase has been considered cubic [Ôsawa, 1929] and [Bowen and Jones, 1931].

Lattice constants of this sample
a = 4.3255(3) Å
c = 5.3465(8)

c/a = 1.2360

Volume
86.6 Å^3

Density
(calculated) 13.827 g/cm^3

Figure of merit
F_{14} = 67.4(0.013,16)

Reference intensity
$I/I_{corundum}$ = 2.34(12)

Polymorphism
SbSn transforms to a different phase at 320 °C [Iwasê et al., 1931].

Additional patterns
1. PDF card 1-830 [Hanawalt et al., 1938]
2. Hägg and Hybinette [1935]

References

Bowen, E. G. and Jones, W. M. (1931). Phil. Mag. 12, 441.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Hägg, G. and Hybinette, A. G. (1935). Phil. Mag. Series 7, 20, 913.
Iwasê, K., Aoki, N., and Ôsawa, A. (1931). Sc. Rep. Tôhoku Imp. Univ. 20, 353.
Ôsawa, A. (1929). Nature 74, 14.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å					
d(Å)	I		hkℓ		2θ(°)
3.067	100	1	0	1	29.09
2.176	30	0	1	2	41.46
2.162	30	1	1	0	41.74
1.7837	8	0	0	3	51.17
1.7679	14	0	2	1	51.66
1.5343	8	2	0	2	60.27
1.3757	8	1	1	3	68.10
1.3683	10	2	1	1	68.52
1.2589	3	1	0	4	75.45
1.2512	7	1	2	2	76.00
1.0878	1	0	2	4	90.16
1.0814	1	2	2	0	90.85
1.0225	2	3	0	3	97.76
1.0200	3	1	3	1	98.09

Barium Bromide Hydrate, $BaBr_2 \cdot 2H_2O$

CAS registry no.
7791-28-8

Sample
The sample was made by slow evaporation of an aqueous solution at room temperature.

Color
Colorless

Optical data
Biaxial (-), N_α = 1.720, N_β = 1.732, N_γ = 1.748. 2V is large.

Structure
Monoclinic, C2/c (15), Z = 4. The structure was determined by Bang [1961].

Lattice constants of this sample
a = 10.442(2) Å
b = 7.207(1)
c = 8.384(2)
β = 113.61(2)°

a/b = 1.4489
c/b = 1.1633

Volume
578.1 $Å^3$

Density
(calculated) 3.828 g/cm^3

Figures of merit
F_{30} = 82.2(0.011,32)
M_{20} = 43.8

Reference intensity
$I/I_{corundum}$ = 4.3(2)

Reference
Bang, E. (1961). Mat. Fys. Medd. Dan. Vid. Selsk. 33, no. 4, 1.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
5.77	25	1 1 0	15.35
5.264	20	-1 1 1	16.83
4.790	2	2 0 0	18.51
4.158	6	1 1 1	21.35
3.842M	30	0 0 2	23.13
3.842M		-2 0 2	23.13
3.623	10	-1 1 2	24.55
3.606	16	0 2 0	24.67
3.265	7	0 2 1	27.29
3.134	1	-3 1 1	28.46
2.937	25	-2 2 1	30.41
2.916	45	3 1 0	30.63
2.890M	100	1 1 2	30.92
2.890M		-3 1 2	30.92
2.629M	11	0 2 2	34.08
2.629M		-2 2 2	34.08
2.582	11	-1 1 3	34.72
2.539M	1	2 0 2	35.32
2.539M		-4 0 2	35.32
2.504	16	2 2 1	35.84
2.446	3	3 1 1	36.71
2.410	6	-3 1 3	37.28
2.391	20	4 0 0	37.58
2.329	3	1 3 0	38.62
2.293	16	-1 3 1	39.26
2.194	3	-2 2 3	41.11
2.171	4	1 3 1	41.57
2.155	2	1 1 3	41.89
2.107	6	-4 2 1	42.89
2.096	14	-2 0 4	43.13
2.085	15	-1 3 2	43.36
1.993	4	4 2 0	45.48
1.981	3	-5 1 1	45.76
1.977	3	-3 3 1	45.86
1.970M	4	-1 1 4	46.03
1.970M		-3 1 4	46.03
1.911+	9	-4 2 3	47.53
1.911+		1 3 2	47.53
1.886	3	-5 1 3	48.22
1.8125M	9	-1 3 3	50.30
1.8125M		-2 2 4	50.30
1.7896	1	4 2 1	50.99
1.7641	2	3 3 1	51.78
1.7407M	8	4 0 2	52.53
1.7407M		-6 0 2	52.53
1.7182	2	2 2 3	53.27
1.7023M	9	1 1 4	53.81
1.7023M		-5 1 4	53.81
1.6858	5	2 4 0	54.38
1.6579	1	5 1 1	55.37

Barium Chlorate, $Ba(ClO_3)_2$

CAS registry no.
13477-00-4

Sample
The sample was prepared by heating $Ba(ClO_3)_2 \cdot H_2O$ at about 250 °C for 15 hours.

Color
Colorless

Structure
Orthorhombic. The crystal system aspect is apparently F*** and Z is assumed to be 8. The cell was determined from the Visser program [1969].

Lattice constants of this sample
a = 11.782(3) Å
b = 13.264(3)
c = 7.727(2)

a/b = 0.8883
c/b = 0.5826

Volume
1207.5 $Å^3$

Density
(calculated) 3.347 g/cm^3 (assuming Z = 8)

Figure of merit
F_{30} = 52.2(0.014,41)

Additional pattern
1. PDF card 1-530 [Hanawalt et al., 1938], data appears to be for $Ba(ClO_4)_2$

References
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Visser, J. W. (1969). J. Appl. Crystallogr. 2, 89.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
5.80	80	1 1 1	15.27
4.401	8	2 2 0	20.16
3.651	60	1 3 1	24.36
3.385	95	3 1 1	26.31
3.337	100	0 2 2	26.69
3.318	45	0 4 0	26.85
3.232	25	2 0 2	27.58
2.945	20	4 0 0	30.33
2.904	9	2 2 2	30.76
2.889	7	2 4 0	30.93
2.745	35	3 3 1	32.59
2.473	20	1 1 3	36.30
2.454	10	1 5 1	36.59
2.314	30	2 4 2	38.88
2.221	13	5 1 1	40.59
2.210M	50	0 6 0	40.80
2.210M		4 2 2	40.80
2.188	14	1 3 3	41.22
2.126	20	3 1 3	42.49
2.114	25	3 5 1	42.73
2.070	8	2 6 0	43.70
2.007	3	5 3 1	45.14
1.936	14	3 3 3	46.89
1.919	12	0 6 2	47.34
1.884	9	6 2 0	48.28
1.8268	9	1 5 3	49.88
1.8200	10	1 7 1	50.08
1.7695	15	2 2 4	51.61
1.7509	5	6 0 2	52.20
1.7239	4	5 1 3	53.08
1.7188	5	5 5 1	53.25
1.6716	11	3 5 3	54.88
1.6685	13	0 4 4	54.99
1.6319	4	7 1 1	56.33
1.6154	4	4 0 4	56.96
1.6081	6	4 6 2	57.24

Barium Iodide Hydrate, $BaI_2 \cdot 2H_2O$

CAS registry no.
7787-33-9

Sample
The sample was made by slow evaporation of an aqueous solution of BaI_2 at about 60 °C.

Color
Strong yellowish brown

Structure
Monoclinic, I2/a (15), Z = 4, by analogy with the powder pattern for $BaBr_2 \cdot 2H_2O$. The axial ratios confirmed those given by Groth [1906]. The equivalent C-centered cell is a = 11.090(2) Å, b = 7.634(1), c = 8.656(2), β = 112.98(2)°.

Lattice constants of this sample

a = 11.089(2) Å
b = 7.634(1)
c = 8.656(2)
β = 112.96(2)°

a/b = 1.4526
c/b = 1.1339

Volume
674.7 $Å^3$

Density
(calculated) 4.206 g/cm^3

Figure of merit
F_{30} = 68.5(0.012,38)

Reference intensity
$I/I_{corundum}$ = 3.4(2)

Reference
Groth, P. (1906). Chemische Krystallographie I (Engelmann, Leipzig, Germany), p. 242.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.12	9	1 1 0	14.47
5.518	16	0 1 1	16.05
5.110	3	2 0 0	17.34
4.386	3	-2 1 1	20.23
3.980M	25	0 0 2	22.32
3.980M		-2 0 2	22.32
3.819	30	0 2 0	23.27
3.765	19	-1 1 2	23.61
3.443	2	-1 2 1	25.86
3.108M	60	3 1 0	28.70
3.108M		1 2 1	28.70
3.058	30	2 2 0	29.18
3.031M	100	1 1 2	29.45
3.031M		-3 1 2	29.45
2.756M	14	0 2 2	32.46
2.756M		-2 2 2	32.46
2.676+	10	-2 1 3	33.46
2.676+		2 0 2	33.46
2.655	13	-3 2 1	33.73
2.599	2	-4 1 1	34.48
2.554	15	4 0 0	35.11
2.468	4	1 3 0	36.37
2.423	12	0 3 1	37.07
2.299	2	-2 3 1	39.16
2.239	3	3 2 1	40.25
2.193+	12	-1 3 2	41.13
2.193+		2 2 2	41.13
2.164	11	-2 0 4	41.71
2.122	5	4 2 0	42.56
2.110	2	4 1 1	42.82
2.039+	3	-1 1 4	44.39
2.039+		-3 1 4	44.39
2.016M	9	1 3 2	44.93
2.016M		-3 3 2	44.93
2.005	6	1 2 3	45.18
1.9735	3	5 1 0	45.95
1.9092	3	0 4 0	47.59
1.9017	5	-5 2 1	47.79
1.8828	7	-2 2 4	48.30
1.8722	2	-4 3 1	48.59
1.8466M	10	4 0 2	49.31
1.8466M		-6 0 2	49.31
1.8068	3	-5 2 3	50.47
1.7972	3	1 4 1	50.76
1.7876	6	2 4 0	51.05
1.7760M	10	1 1 4	51.41
1.7760M		-5 1 4	51.41
1.7657+	5	0 2 4	51.73
1.7657+		-4 2 4	51.73
1.7364	1	-6 1 3	52.67
1.7011	1	6 0 0	53.85
1.6953	4	-3 4 1	54.05
1.6621+	14	4 2 2	55.22
1.6621+		-6 2 2	55.22
1.6505M	4	2 0 4	55.64
1.6505M		-6 0 4	55.64
1.6389M	1	5 2 1	56.07
1.6389M		-4 1 5	56.07
1.6156	1L	3 2 3	56.95
1.5921	5	5 3 0	57.87
1.5706	1	3 4 1	58.74
1.5531+	6	6 2 0	59.47
1.5531+		2 4 2	59.47
1.5500+	5	5 1 2	59.60
1.5500+		-7 1 2	59.60

Barium Phosphate, $Ba_2P_2O_7$, (high form)

CAS registry no.
13466-21-2

Sample
The sample was prepared by heating $BaCO_3$ with $H_4P_2O_7$ at 950 °C for 1 hour, grinding and heating a few minutes at 1100 °C. Chemical analysis of material dried at 100 °C gave BaO as 68.25 percent and P_2O_5 as 31.12 percent. The theoretical composition for $Ba_2P_2O_7$ gives BaO = 68.4 percent and P_2O_5 = 31.6 percent.

Color
Colorless

Optical data
Uniaxial (+), N_o = 1.595, N_e = 1.600

Structure
Hexagonal. The crystal system aspect is apparently $P6_3$** and Z is assumed to be 3. The cell was determined from the Visser [1969] program. Ranby et al. [1955] proposed an orthorhombic cell for this phase. It did not fit our data. Mehdi et al. [1977] proposed a different orthorhombic cell which did not properly fit his data or ours.

Lattice constants of this sample
a = 9.4175(8) Å
c = 7.081(1)

c/a = 0.7519

Volume
543.85 Å^3

Density
(calculated) 4.109 g/cm^3, assuming Z = 3.

Figures of merit
F_{30} = 54.8(0.012,46)
M_{20} = 58.7

Reference intensity
$I/I_{corundum}$ = 4.3(2)

Polymorphism
Below about 725 °C, $Ba_2P_2O_7$ forms an α phase, isostructural with α-$Ca_2P_2O_7$ [McCauley and Hummel, 1968; Ranby et al., 1955].

Additional patterns
1. PDF card 9-45 [Langguth et al., 1956]
2. Mehdi et al. [1977]
3. Ranby et al. [1955]

References

Langguth, R. P., Osterheld, R. K., and Karl-Kroupa, E. (1956). J. Phys. Chem. 60, 1335.
McCauley, R. A. and Hummel, F. A. (1968). Trans. Brit. Ceram. Soc. 67, 624.
Mehdi, S., Hussain, M. R., and Rao, B. R. (1977). Indian J. Chem. 15A, 820.
Ranby, P. W., Mash, D. H., and Henderson, S. T. (1955). Brit. J. Appl. Phys. 6, Sup 4, S18.
Visser, J. W. (1969). J. Appl. Crystallogr. 2, 89.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
5.346	4	1 0 1	16.57
4.709	1	1 1 0	18.83
3.923	100	1 1 1	22.65
3.539	25	0 0 2	25.14
3.084	7	2 1 0	28.93
2.833	35	1 1 2	31.56
2.719	25	3 0 0	32.91
2.355	16	2 2 0	38.18
2.325	20	2 1 2	38.69
2.262	10	3 1 0	39.82
2.235	13	2 2 1	40.33
2.156M	18	3 0 2	41.87
2.156M		3 1 1	41.87
2.110	17	1 1 3	42.82
2.043	40	2 0 3	44.30
2.038	40	4 0 0	44.42
1.960M	7	2 2 2	46.28
1.960M		4 0 1	46.28
1.907	3	3 1 2	47.66
1.8711	4	3 2 0	48.62
1.8092	7	3 2 1	50.40
1.7705	5	0 0 4	51.58
1.7258	3	4 1 1	53.02
1.6671	2	2 2 3	55.04
1.6338	4	3 1 3	56.26
1.5896M	5	4 1 2	57.97
1.5896M		5 0 1	57.97
1.5694	1	3 3 0	58.79
1.5415	5	4 2 0	59.96
1.5327	3	3 3 1	60.34
1.5055	1L	4 2 1	61.55
1.4829	4	3 0 4	62.59
1.4653	3	5 1 0	63.43
1.4340	4	5 1 1	64.98
1.4210	3	4 1 3	65.65
1.4130	3	4 2 2	66.07
1.3938	1	3 1 4	67.10
1.3540	3	5 1 2	69.35
1.3413M	1	5 0 3	70.10
1.3413M		4 3 0	70.10
1.3380	2	2 0 5	70.30
1.3170	2	4 3 1	71.59
1.2903	1	4 2 3	73.31
1.2856	2	3 2 4	73.62

Barium Thiosulfate Hydrate, $BaS_2O_3 \cdot H_2O$

CAS registry no.
13466-25-6

Sample
The sample was made by adding a concentrated solution of $Na_2S_2O_3$ to a similar hot solution of $BaCl_2$. The solution was then cooled. This produced small plates. When the pure material was dissolved in water and the liquid allowed to evaporate at room temperature, small needles were formed. The intensities were determined on a mixture of the crystal types.

Color
Colorless

Structure
Orthorhombic, Pnca (60), Z = 8. The structure of $BaS_2O_3 \cdot H_2O$ was studied by Nardelli and Fava [1962].

Lattice constants of this sample
a = 7.386(1) Å
b = 20.050(3)
c = 7.191(2)

a/b = 0.3684
c/b = 0.3587

Volume
1064.9 $Å^3$

Density
(calculated) 3.337 g/cm^3

Figure of merit
F_{30} = 51.4 (0.015,40)

Additional pattern
1. PDF card 1-42 [Hanawalt et al., 1938]

References
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Nardelli, M. and Fava, G. (1962). Acta Crystallogr. 15, 477.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
10.04	9	0 2 0	8.80
5.018	60	0 4 0	17.66
4.900	7	0 3 1	18.09
4.588	35	1 2 1	19.33
4.085	5	1 3 1	21.74
3.694	50	2 0 0	24.07
3.630	50	2 1 0	24.50
3.594M	100	0 0 2	24.75
3.594M		1 4 1	24.75
3.501	10	0 5 1	25.42
3.468	20	2 2 0	25.67
3.386	25	0 2 2	26.30
3.342	75	0 6 0	26.65
3.244	11	2 1 1	27.47
3.235M	16	1 0 2	27.55
3.235M		2 3 0	27.55
3.190	25	1 1 2	27.95
3.162	5	1 5 1	28.20
3.077	8	1 2 2	29.00
2.973	16	2 4 0	30.03
2.922	25	0 4 2	30.57
2.748	10	2 4 1	32.56
2.715M	12	1 4 2	32.97
2.715M		2 5 0	32.97
2.661	11	0 7 1	33.65
2.577	35	2 0 2	34.78
2.554	30	2 1 2	35.11
2.508	30	0 8 0	35.78
2.479	55	2 6 0	36.21
2.449	55	0 6 2	36.66
2.382	6	0 1 3	37.73
2.343	6	2 6 1	38.39
2.314	16	3 1 1	38.88
2.292	20	2 4 2	39.28
2.263	45	2 7 0	39.80
2.254M	55	1 8 1	39.96
2.254M		0 3 3	39.96
2.223	30	1 2 3	40.55
2.199	18	3 3 1	41.01
2.166	14	2 5 2	41.66
2.146	10	1 7 2	42.08
2.128	2	0 9 1	42.45
2.112	7	3 4 1	42.78
2.076	15	1 4 3	43.56
2.057M	10	0 5 3	43.99
2.057M		0 8 2	43.99
2.040	35	2 6 2	44.38
2.006	9	0 10 0	45.17
1.916	11	2 7 2	47.40
1.869	12	1 10 1	48.69
1.847	5	4 0 0	49.31
1.839M	8	4 1 0	49.54
1.839M		0 7 3	49.54
1.8071	7	3 7 1	50.46
1.7619	12	2 10 0	51.85
1.7512	11	0 10 2	52.19
1.7401	8	1 1 4	52.55
1.7355	7	3 6 2	52.70
1.6863	6	1 8 3	54.36
1.6707	12	0 12 0	54.91
1.6341M	18	2 11 0	56.25
1.6341M		4 5 1	56.25
1.6159M	10	2 0 4	56.94
1.6159M		4 6 0	56.94
1.6102	12	3 9 1	57.16

d(Å)	I	hkℓ	2θ(°)
1.6010	10	1 5 4	57.52
1.5824M	18	0 6 4	58.26
1.5824M		2 10 2	58.26
1.5514	7	4 7 0	59.54
1.5220	18	2 12 0	60.81
1.5146	17	0 12 2	61.14
1.4876	8	2 11 2	62.37
1.4229M	14	1 11 3	65.55
1.4229M		2 13 0	65.55

o-Bromobenzoic Acid, $C_7H_5BrO_2$

Synonym
1. 2-Bromobenzoic Acid

CAS registry no.
88-65-3

Sample
The sample was NBS Standard Reference Material 2142.

Color
Colorless

Structure
Monoclinic, A2/a (15), Z = 8. The structure was determined by Ferguson and Sim [1962].

Lattice constants of this sample
a = 23.016(4) Å
b = 4.085(1)
c = 14.871(3)
β = 96.62(2)°

a/b = 5.6343
c/b = 3.6404

Volume
1389.0 Å^3

Density
(calculated) 1.923 g/cm^3

Figure of merit
F_{30} = 68.6(0.012,37)

Reference intensity
$I/I_{corundum}$ = 0.80(2)

Additional pattern
1. PDF card 13-794 [Ferguson and Sim, 1959]

Reference
Ferguson, G. and Sim, G. A. (1962). Acta Crystallogr. 15, 346.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
11.41	13	2 0 0	7.74
7.41	5	0 0 2	11.94
6.56	55	-2 0 2	13.49
5.905	80	2 0 2	14.99
5.716	25	4 0 0	15.49
4.805	4	-4 0 2	18.45
4.290	40	4 0 2	20.69
3.940	30	0 1 1	22.55
3.862	60	1 1 1	23.01
3.811	40	6 0 0	23.32
3.756	25	-2 1 1	23.67
3.691M	90	0 0 4	24.09
3.691M		2 1 1	24.09
3.641	45	-2 0 4	24.43
3.558	65	-6 0 2	25.01
3.454	19	3 1 1	25.77
3.401	18	2 0 4	26.18
3.288	100	-4 1 1	27.10
3.237	14	6 0 2	27.53
3.198	30	4 1 1	27.88
3.144M	5	0 1 3	28.36
3.144M		-1 1 3	28.36
3.088M	17	-2 1 3	28.89
3.088M		1 1 3	28.89
3.033	6	-5 1 1	29.43
2.982	20	-3 1 3	29.94
2.974	17	2 1 3	30.02
2.950	12	4 0 4	30.27
2.856	40	8 0 0	31.29
2.781	19	-6 1 1	32.16
2.696	11	6 1 1	33.20
2.673	25	4 1 3	33.50
2.569	14	8 0 2	34.90
2.511	30	6 0 4	35.73
2.465	19	-2 0 6	36.42
2.388	25	-2 1 5	37.63
2.352M	9	2 0 6	38.23
2.352M		-7 1 3	38.23
2.347M	7	-8 1 1	38.32
2.347M		-3 1 5	38.32
2.300	6	2 1 5	39.13
2.280	19	8 1 1	39.49
2.259	4	-10 0 2	39.87
2.226	4	3 1 5	40.49
2.186M	8	7 1 3	41.26
2.186M		-6 0 6	41.26
2.139	9	4 1 5	42.22
2.115	6	10 0 2	42.71
2.106	6	9 1 1	42.91
2.052M	8	-9 1 3	44.10

d(Å)	I	hkℓ			2θ(°)
2.052M		-10	0	4	44.10
1.981	5	-8	0	6	45.76
1.967M	18	-1	2	2	46.12
1.967M		6	0	6	46.12
1.950M	11	-2	2	2	46.54
1.950M		10	1	1	46.54
1.9264	10	-8	1	5	47.14
1.9237	9	4	2	0	47.21
1.9047	4	12	0	0	47.71
1.8835	11	-1	1	7	48.28
1.8751	9	0	1	7	48.51
1.8568	5	-2	0	8	49.02
1.8497M	5	7	1	5	49.22
1.8497M		10	0	4	49.22
1.8385	5	-4	1	7	49.54
1.8282M	7	-5	2	2	49.84
1.8282M		-9	1	5	49.84
1.8200M	8	-4	0	8	50.08
1.8200M		2	1	7	50.08
1.8005M	6	6	2	0	50.66
1.8005M		-5	1	7	50.66
1.7955M	10	12	0	2	50.81
1.7955M		-11	1	3	50.81
1.7880+	12	10	1	3	51.04
1.7880+		5	2	2	51.04
1.7670	8	8	0	6	51.69
1.7559M	6	8	1	5	52.04
1.7559M		-6	1	7	52.04

Cadmium Borate, CdB_4O_7

Sample
The sample was prepared by heating CdO and B_2O_3 in a 1:2 molar mixture at 900 °C for 5 hours.

Color
Colorless

Structure
Orthorhombic, Pbca (61), Z = 8, [Hand and Krogh-Moe, 1962]. The structure of CdB_4O_7 has been determined by Ihara and Krogh-Moe [1966].

Lattice constants of this sample
a = 8.704(1) Å
b = 14.176(2)
c = 8.229(1)

a/b = 0.6140
c/b = 0.5805

Volume
1015.4 $Å^3$

Density
(calculated) 3.501 g/cm^3

Figure of merit
F_{30} = 50.8(0.013,46)

Reference intensity
$I/I_{corundum}$ = 0.82(6)

Additional pattern
1. PDF card 14-162 [Hand and Krogh-Moe, 1962]

References
Hand, D. and Krogh-Moe, J. (1962). J. Amer. Ceram. Soc. 45, 197.
Ihara,M. and Krogh-Moe, J. (1966). Acta Crystallogr. 20, 132.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
7.10	12	0 2 0	12.45
5.504	70	1 1 1	16.09
5.371	100	0 2 1	16.49
4.574	11	1 2 1	19.39
4.164	50	2 1 0	21.32
4.113	30	0 0 2	21.59
3.717M	80	1 0 2	23.92
3.717M		2 1 1	23.92
3.599	60	1 1 2	24.72
3.555	45	0 2 2	25.03
3.544	45	0 4 0	25.11
3.202	95	2 3 0	27.84
2.984	30	2 3 1	29.92
2.924M	70	2 1 2	30.55
2.924M		1 3 2	30.55
2.749	20	2 4 0	32.54
2.687M	19	3 1 1	33.32
2.687M		0 4 2	33.32
2.559	85	0 2 3	35.04
2.527	2	2 3 2	35.49
2.456	13	1 2 3	36.56
2.372	25	3 0 2	37.90
2.338	5	3 1 2	38.47
2.290M	40	2 1 3	39.32
2.290M		1 3 3	39.32
2.282	60	2 5 1	39.45
2.272	20	0 6 1	39.63
2.255	8	1 5 2	39.95
2.197	10	1 6 1	41.04
2.176	25	4 0 0	41.46
2.120	4	3 3 2	42.61
2.082M	6	2 3 3	43.42
2.082M		4 1 1	43.42
2.059M	16	2 5 2	43.94
2.059M		0 0 4	43.94
2.016	30	4 2 1	44.93
1.994	5	1 6 2	45.46
1.970M	55	3 4 2	46.03
1.970M		3 5 1	46.03
1.918M	14	3 2 3	47.35
1.918M		1 7 1	47.35
1.8540M	20	4 4 0	49.10
1.8540M		2 6 2	49.10
1.8438M	20	2 1 4	49.39
1.8438M		1 3 4	49.39
1.8361M	30	3 3 3	49.61
1.8361M		2 7 0	49.61
1.7958	30	2 5 3	50.80
1.7916	20	2 7 1	50.93
1.7785M	30	0 4 4	51.33
1.7785M		1 7 2	51.33
1.7718	20	0 8 0	51.54
1.7531	4	1 6 3	52.13
1.7435	2	1 4 4	52.44
1.7306	25	2 3 4	52.86
1.6988	4	1 8 1	53.93
1.6912M	8	5 1 1	54.19
1.6912M		4 4 2	54.19
1.6744	8	3 6 2	54.78
1.6577	18	4 2 3	55.38
1.6274M	3	3 7 1	56.50
1.6274M		0 8 2	56.50
1.6066	7	1 1 5	57.30
1.6023	9	5 3 1	57.47
1.6002M	11	4 6 0	57.55

d(Å)	I	hkℓ	2θ(°)
1.6002M		1 8 2	57.55
1.5926M	7	5 1 2	57.85
1.5926M		4 5 2	57.85
1.5765	5	1 2 5	58.50
1.5706	10	4 6 1	58.74
1.5552	5	2 5 4	59.38
1.5512	4	0 6 4	59.55
1.5399	4	3 7 2	60.03
1.5302M	6	2 1 5	60.45
1.5302M		1 3 5	60.45
1.5234M	11	3 6 3	60.75
1.5234M		1 9 1	60.75
1.5188	13	5 3 2	60.95
1.4943	5	4 0 4	62.06
1.4876M	7	0 8 3	62.37
1.4876M		3 8 1	62.37
1.4624M	11	4 2 4	63.57
1.4624M		5 1 3	63.57
1.4601M	15	5 4 2	63.68
1.4601M		5 5 1	63.68
1.4428	3	6 1 0	64.54
1.4208M	6	6 2 0	65.66
1.4208M		3 7 3	65.66
1.4176	7	0 10 0	65.83
1.4032M	10	5 3 3	66.59
1.4032M		3 2 5	66.59
1.3958	4	5 5 2	66.99
1.3869	5	6 3 0	67.48
1.3818M	7	4 6 3	67.76
1.3818M		5 6 1	67.76
1.3777	10	4 4 4	67.99
1.3740	9	4 8 0	68.20
1.3699M	14	3 3 5	68.43
1.3699M		2 7 4	68.43

Cadmium Phosphate, $Cd_2P_2O_7$

Sample
The sample was prepared by heating a 1:1 molar mixture of $CdCO_3$ and $(NH_4)_2HPO_4$ at 700 °C for several days, followed by heating at 800 °C for 2 hours.

Color
Colorless

Structure
Triclinic, $P\bar{1}$ (2), Z = 2. The structure of $Cd_2P_2O_7$ was determined by Calvo and Au [1969].

Lattice constants of this sample
a = 6.602(2) Å
b = 6.778(2)
c = 6.631(2)
α = 95.79(2)°
β = 97.68(2)
γ = 65.00(2)

a/b = 0.9740
c/b = 0.9783

Volume
266.2 Å^3

Density
(calculated) 4.975 g/cm^3

Figure of merit
F_{30} = 51.3(0.012,47)

Reference intensity
$I/I_{corundum}$ = 1.58(3)

Additional patterns
1. PDF card 17-635 [Brown and Hummel, 1964]
2. Ropp et al. [1961]

References
Brown, J. J. and Hummel, F. A. (1964). J. Electrochem. Soc. 111, 1052.
Calvo, C. and Au, P. K. L. (1969). Can. J. Chem. 47, 3409.
Ropp, R. C., Mooney, R. W., and Hoffman, C. W. W. (1961). Anal. Chem. 33, 1687.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.15	12	0 1 0	14.40
5.965	8	1 0 0	14.84
4.645	11	-1 0 1	19.09
4.586	18	-1 -1 1	19.34
4.377	15	0 1 1	20.27
4.207	40	1 0 1	21.10
3.987	14	1 1 1	22.28
3.353	30	1 2 0	26.56
3.279	25	0 0 2	27.17
3.262	35	2 1 0	27.32
3.194	35	-1 1 1	27.91
3.126	35	-1 -2 1	28.53
3.094	100	-2 -1 1	28.83
3.068	85	0 2 0	29.08
2.974	45	2 0 0	30.02
2.956	80	0 -1 2	30.21
2.835M	90	0 1 2	31.53
2.835M		0 -2 1	31.53
2.794	7	2 2 0	32.01
2.729	8	0 2 1	32.79
2.708	5	-2 -2 1	33.05
2.671	10	1 1 2	33.53
2.613	20	2 0 1	34.29
2.489	14	-2 -1 2	36.05
2.449	30	2 2 1	36.66
2.325M	30	-2 1 0	38.69
2.325M		-2 0 2	38.69
2.298	14	0 -2 2	39.17
2.240	4	1 3 0	40.23
2.218	20	1 -2 1	40.65
2.187M	6	0 2 2	41.25
2.187M		0 0 3	41.25
2.170M	30	3 1 0	41.58
2.170M		2 1 2	41.58
2.142	16	-1 -1 3	42.16
2.124	30	-1 0 3	42.52
2.114	17	3 2 0	42.73
2.101M	12	2 0 2	43.01
2.101M		-3 -2 1	43.01
1.993	6	2 2 2	45.47
1.974	4	2 3 1	45.93
1.9526	14	-2 1 2	46.47
1.9470	16	1 1 3	46.61
1.9256M	18	0 3 1	47.16
1.9256M		-3 -1 2	47.16
1.8961	4	-1 1 3	47.94
1.8526	18	-2 -2 3	49.14
1.7756M	14	0 -3 2	51.42
1.7756M		1 3 2	51.42
1.7264M	14	-1 3 0	53.00
1.7264M		-3 -3 2	53.00
1.7117M	14	2 1 3	53.49
1.7117M		3 1 2	53.49
1.6982	8	0 3 2	53.95

Cadmium Phosphate, $Cd_3(PO_4)_2$

Sample
The sample was prepared by heating a 3:2 molar mixture of CdO and $(NH_4)_2HPO_4$ at 800 °C overnight.

Color
Colorless

Structure
Monoclinic, $P2_1/c$ (14), Z = 4. The cell was found by use of the Visser program [1969] and by comparison with β-$Zn_3(PO_4)_2$ and $Mn_3(PO_4)_2$. The space group was assigned by consideration of the absences in the powder pattern.

Lattice constants of this sample
a = 8.662(2) Å
b = 10.333(3)
c = 8.307(2)
β = 114.48(2)°

a/b = 0.8383
c/b = 0.8039

Volume
676.7 Å^3

Density
(calculated) 5.174 g/cm^3 (assuming Z = 4)

Figures of merit
F_{30} = 72.4(0.011,39)
M_{20} = 35.5

Reference intensity
$I/I_{corundum}$ = 1.16(6)

Additional pattern
1. PDF card 14-443 [Ropp et al., 1962]

References
Ropp, R. C., Mooney, R. W., and Hoffman, C. W. W. (1961). Anal. Chem. 33, 1687.
Visser, J. W. (1969). J. Appl. Crystallogr. 2, 89.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
7.87	2	1 0 0	11.23
6.27	4	1 1 0	14.12
6.10	6	0 1 1	14.50
4.318	50	1 2 0	20.55
4.263	25	0 2 1	20.82
4.195	14	1 1 1	21.16
3.969	25	-2 1 1	22.38
3.942	9	2 0 0	22.54
3.844	30	-1 1 2	23.12
3.778	19	0 0 2	23.53
3.562	30	-2 0 2	24.98
3.429	80	1 2 1	25.96
3.367	90	-2 1 2	26.45
3.305	100	-2 2 1	26.96
3.230	18	-1 2 2	27.59
3.154	60	1 3 0	28.27
3.101	25	-1 3 1	28.77
3.051	30	0 2 2	29.25
2.962	85	1 0 2	30.15
2.933	16	-2 2 2	30.45
2.898	35	2 1 1	30.83
2.848	18	1 1 2	31.38
2.775	3	-3 1 1	32.23
2.753	3	1 3 1	32.50
2.663M	45	-1 1 3	33.63
2.663M		-3 1 2	33.63
2.650	50	-1 3 2	33.80
2.627	30	3 0 0	34.10
2.594	45	2 3 0	34.55
2.546M	8	0 3 2	35.22
2.546M		3 1 0	35.22
2.516	18	-3 2 1	35.65
2.477	4	-2 3 2	36.24
2.449	25	0 1 3	36.66
2.431M	25	-1 2 3	36.94
2.431M		-3 2 2	36.94
2.385	2	-2 2 3	37.69
2.317	4	-3 1 3	38.84
2.270	4	2 3 1	39.67
2.265	3	0 2 3	39.76
2.251	1L	1 4 1	40.02
2.213	3	-2 4 1	40.74
2.152M	12	-1 3 3	41.95
2.152M		-4 0 2	41.95
2.106	12	-4 1 2	42.91
2.099	10	2 2 2	43.05
2.092M	12	-2 4 2	43.20
2.092M		-4 1 1	43.20
2.073	3	-2 0 4	43.63
2.034M	16	0 3 3	44.51
2.034M		3 2 1	44.51
1.994	15	0 5 1	45.45
1.987	16	-4 2 2	45.63
1.971M	25	-4 1 3	46.00
1.971M		4 0 0	46.00
1.936M	17	4 1 0	46.90
1.936M		-3 1 4	46.90
1.923M	13	-3 4 1	47.23
1.923M		-2 2 4	47.23
1.910	25	2 3 2	47.57
1.885M	15	1 5 1	48.24
1.885M		-1 4 3	48.24
1.8632M	8	-2 5 1	48.84
1.8632M		-2 4 3	48.84
1.8424M	12	3 4 0	49.43
1.8424M		4 2 0	49.43

Calcium Aluminum Iron Oxide (Brownmillerite), $Ca_4Al_2Fe_2O_{10}$

CAS registry no.
12068-35-8

Sample
The sample was prepared by the Portland Cement Association. This phase is a component of portland cement and is known as C_4AF.

Color
Deep brown

Structure
Orthorhombic, Pcmn (62), Z = 2. The structure was determined by Bertaut et al. [1959]. $Ca_4Al_2Fe_2O_{10}$ is isostructural and forms a series of solid solutions with $Ca_2Fe_2O_5$ [Bertaut et al., 1959].

Lattice constants of this sample
a = 5.5672(9) Å
b = 14.521(2)
c = 5.349(1)

a/b = 0.3834
c/b = 0.3684

Volume
432.4 $Å^3$

Density
(calculated) 3.732 g/cm^3

Figure of merit
F_{30} = 30.9(0.011,85)

Reference intensity
$I/I_{corundum}$ = 1.32(10)

Additional patterns
1. PDF card 11-124 [Midgley, 1957]
2. Bertaut et al. [1959]
3. Hansen et al. [1928]

References

Bertaut, E. F., Blum, P., and Sagnieres, A. (1959). Acta Crystallogr. 12, 149.
Hansen, W. C. and Brownmiller, S. T. (1928). Amer. J. Sci. 15, 224.
Midgley, H. G. (1957). Mag. Concr. Res. March 1957.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
7.25	45	0 2 0	12.20
5.193	4	1 1 0	17.06
3.859	4	1 0 1	23.03
3.654	16	1 3 0	24.34
3.629	6	0 4 0	24.51
3.406	4	1 2 1	26.14
2.784	25	2 0 0	32.12
2.673	35	0 0 2	33.50
2.644	100	1 4 1	33.88
2.576	17	1 5 0	34.80
2.472	2	2 0 1	36.32
2.434	4	2 1 1	36.90
2.210	8	2 4 0	40.79
2.155	9	0 4 2	41.89
2.051	35	1 6 1	44.13
1.9283	35	2 0 2	47.09
1.8813	3	2 5 1	48.34
1.8632	9	2 2 2	48.84
1.8149	45	0 8 0	50.23
1.7952	3	0 6 2	50.82
1.7327	7	3 3 0	52.79
1.5784	14	3 4 1	58.42
1.5638	4	3 5 0	59.02
1.5380	14	1 4 3	60.11
1.5202	7	2 8 0	60.89
1.5013+	8	2 0 3	61.74
1.5013+		3 5 1	61.74
1.4524	4	0 10 0	64.06
1.4197	5	3 6 1	65.72
1.3901	6	1 6 3	67.30
1.3669	3	4 2 0	68.60
1.3588	5	1 10 1	69.07
1.3373	4	0 0 4	70.34
1.3215	12	2 8 2	71.31

Calcium Boride, CaB_6

CAS registry no.
12007-99-7

Sample
The sample was obtained from Alfa Products (Ventron), Danvers, MA.

Color
Dark olive brown

Structure
Cubic, Pm3m (221), Z = 1. The structure was determined by von Stackelberg and Newmann [1932].

Lattice constant of this sample
a = 4.1535(1) Å

Volume
71.653 Å^3

Density
(calculated) 2.432 g/cm^3

Figure of merit
F_{21} = 74.2(0.012,24)

Reference intensity
$I/I_{corundum}$ = 1.92(10)

Additional pattern
1. PDF card 3-654 [von Stackelberg and Neumann, 1932].

Reference
von Stackelberg, M. and Neumann, F. (1932). Z. Phys. Chem. 19, 314.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
4.151	6	1 0 0	21.39
2.938	100	1 1 0	30.40
2.398	45	1 1 1	37.48
2.077	25	2 0 0	43.53
1.8572	30	2 1 0	49.01
1.6953	5	2 1 1	54.05
1.4686	3	2 2 0	63.27
1.3847	19	3 0 0	67.60
1.3137	13	3 1 0	71.80
1.2523	4	3 1 1	75.92
1.1522	1	3 2 0	83.91
1.1100	4	3 2 1	87.89
1.0384	2	4 0 0	95.77
1.0073	3	4 1 0	99.76
.9791	4	4 1 1	103.76
.9528	1L	3 3 1	107.89
.9287	2	4 2 0	112.09
.9064	4	4 2 1	116.38
.8856	2	3 3 2	120.87
.8146	4	5 1 0	142.05
.7993	3	5 1 1	149.04

m-Chlorobenzoic Acid, $C_7H_5ClO_2$

Synonym
1. 3-Chlorobenzoic Acid

CAS registry no.
535-80-8

Sample
The sample was NBS Standard Reference Material 2144.

Color
Colorless

Structure
Monoclinic, $P2_1/a$ (14), Z = 4. The structure was determined by Gougoutas and Lessinger [1975].

Lattice constants of this sample
a = 11.110(2) Å
b = 16.015(3)
c = 3.8455(8)
β = 95.00(2)°

a/b = 0.6937
c/b = 0.2401

Volume
681.6 Å^3

Density
(calculated) 1.526 g/cm^3

Figure of merit
F_{30} = 53.8(0.011,52)

Reference intensity
$I/I_{corundum}$ = 0.63(7)

Additional patterns
1. PDF card 24-1594 [Li, Polytechnic Institute of Brooklyn, Brooklyn, NY.]
2. PDF card 20-1577 [Dept. of Physics, Univ. Coll., Cardiff, Wales.]

Reference
Gougoutas, J. Z. and Lessinger, L. (1975). J. Solid State Chem. 12, 51.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
9.07	6	1 1 0	9.74
6.48	85	1 2 0	13.65
5.538	7	2 0 0	15.99
4.808	55	1 3 0	18.44
4.549	16	2 2 0	19.50
4.005	18	0 4 0	22.18
3.842	45	2 3 0	23.13
3.622	45	-1 1 1	24.56
3.591	16	3 1 0	24.77
3.453	35	0 2 1	25.78
3.376	100	-1 2 1	26.38
3.351	14	3 2 0	26.58
3.287	75	-2 0 1	27.11
3.243	95	2 4 0	27.48
3.220	90	-2 1 1	27.68
3.114	9	0 3 1	28.64
3.077	12	1 5 0	29.00
3.041	5	-2 2 1	29.35
2.799	10	-2 3 1	31.95
2.771M	10	2 5 0	32.28
2.771M		0 4 1	32.28
2.727M	8	4 1 0	32.82
2.727M		-1 4 1	32.82
2.670	12	0 6 0	33.54
2.629	4	-3 2 1	34.07
2.615	4	4 2 0	34.26
2.516	8	3 1 1	35.65
2.456M	20	4 3 0	36.56
2.456M		0 5 1	36.56
2.416M	25	2 4 1	37.18
2.416M		3 5 0	37.18
2.342	2	-4 0 1	38.41
2.301	4	3 3 1	39.11
2.276	5	4 4 0	39.57
2.240	1	1 7 0	40.23
2.201	2	2 5 1	40.98
2.192	3	5 1 0	41.14
2.168	8	-1 6 1	41.63
2.162	9	3 6 0	41.74
2.156	8	4 0 1	41.87
2.134	7	5 2 0	42.31
2.113	3	2 7 0	42.75
2.044	4	5 3 0	44.27
2.002M	13	2 6 1	45.25
2.002M		0 8 0	45.25
1.971	2	1 8 0	46.02
1.9376	2	5 4 0	46.85
1.9214	2	4 6 0	47.27
1.8983	3	4 4 1	47.88
1.8788	6	-2 7 1	48.41
1.8326	2	6 1 0	49.71
1.7635+	9	2 0 2	51.80
1.7635+		4 7 0	51.80
1.7597M	9	3 8 0	51.92
1.7597M		-4 6 1	51.92
1.7432	7	6 3 0	52.45
1.6930M	7	-5 5 1	54.13
1.6930M		2 9 0	54.13
1.6747+	4	-3 3 2	54.77
1.6747+		2 3 2	54.77

Chromium Chloride Hydrate, $CrCl_3 \cdot 6H_2O$

Synonym
1. Dichlorotetraaquochromium(III) chloride dihydrate, $[Cr(H_2O)_4Cl_2]Cl \cdot 2H_2O$

CAS registry no.
10060-12-5

Sample
The sample was obtained from City Chemical Corp., New York, NY.

Color
Very dark yellowish green

Structure
Monoclinic, C2/c (15), Z = 4. The structure was determined by Dance and Freeman [1965]. Morosin [1966] had also independently determined the same structure. The synonym name and formula are those obtained as the results of crystal structure analysis.

Lattice constants of this sample

a = 12.048(2) Å
b = 6.8352(8)
c = 11.643(1)
β = 94.14(1)°

a/b = 1.7626
c/b = 1.7032

Volume
956.27 Å^3

Density
(calculated) 1.851 g/cm^3

Figure of merit
F_{30} = 65.2(0.012,39)

Polymorphism
A hexagonal modification has been reported by Andress and Carpenter [1934].

Additional pattern
1. PDF card 12-446 [Shrier, Rutgers University]

References
Andress, K. R. and Carpenter, C. (1934) Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 87A, 446.
Dance, I. G. and Freeman, H. C. (1965). J. Inorg. Chem. 4, 1555.
Morosin, B. (1966). Acta Crystallogr. 21, 280.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
6.00	45	2 0 0	14.74
5.805	30	0 0 2	15.25
5.362	100	-1 1 1	16.52
5.211	65	1 1 1	17.00
4.333	30	-2 0 2	20.48
4.079	18	1 1 2	21.77
4.032	16	2 0 2	22.03
3.456	30	3 1 0	25.76
3.371	55	-3 1 1	26.42
3.297	25	-1 1 3	27.02
3.278	30	0 2 1	27.18
3.054	40	-3 1 2	29.22
3.006	6	4 0 0	29.70
2.946	40	0 2 2	30.32
2.902M	17	-2 2 1	30.79
2.902M		0 0 4	30.79
2.893	14	3 1 2	30.88
2.853	13	2 2 1	31.33
2.749	19	-4 0 2	32.54
2.690	30	-2 0 4	33.28
2.682	25	-2 2 2	33.38
2.644	6	-1 1 4	33.87
2.605	25	2 2 2	34.40
2.592	30	4 0 2	34.58
2.571	40	1 1 4	34.87
2.543	9	2 0 4	35.27
2.500	8	3 1 3	35.89
2.398	8	-2 2 3	37.48
2.294	2	-3 1 4	39.24
2.268	3	5 1 0	39.71
2.256M	6	4 2 0	39.93
2.256M		-5 1 1	39.93
2.238M	6	-4 2 1	40.27
2.238M		1 3 0	40.27
2.212	5	0 2 4	40.76
2.204	5	-1 3 1	40.91
2.194M	9	4 2 1	41.11
2.194M		1 3 1	41.11
2.189	8	-1 1 5	41.20
2.167	8	-4 0 4	41.64
2.138	15	1 1 5	42.24
2.115	3	-2 2 4	42.71
2.080	2	1 3 2	43.47
2.066M	7	4 2 2	43.78
2.066M		5 1 2	43.78
2.040	20	2 2 4	44.36
2.017M	10	-5 1 3	44.91
2.017M		4 0 4	44.91
1.997	4	-4 2 3	45.37
1.980	3	3 3 0	45.78

d(Å)	I	hkℓ			2θ(°)
1.949	8	-1	3	3	46.56
1.940	25	3	3	1	46.79
1.936M	30	-6	0	2	46.88
1.936M		0	0	6	46.88
1.9268	17	1	3	3	47.13
1.9047	6	4	2	3	47.71
1.9006	4	5	1	3	47.82
1.8824	8	-2	0	6	48.31
1.8748	7	3	1	5	48.52
1.8600	9	-1	1	6	48.93
1.8547	8	3	3	2	49.08
1.8299	2	-4	2	4	49.79
1.8048	10	2	0	6	50.53
1.7893	7	-3	3	3	51.00
1.7379M	5	3	3	3	52.62
1.7379M		4	2	4	52.62
1.7349	6	-3	1	6	52.72
1.7282	14	6	2	0	52.94
1.7084M	2	0	4	0	53.60
1.7084M		-6	0	4	53.60
1.6907	6	0	4	1	54.21
1.6843+	5	0	2	6	54.43
1.6843+		-6	2	2	54.43
1.6643+	5	-7	1	1	55.14
1.6643+		-4	2	5	55.14
1.6454	3	3	1	6	55.83
1.6394	4	0	4	2	56.05
1.6266	7	5	3	1	56.53
1.6235M	7	2	4	1	56.65
1.6235M		-1	3	5	56.65
1.6130	4	-1	1	7	57.05
1.5962M	3	2	2	6	57.71
1.5962M		6	0	4	57.71
1.5836	3	1	1	7	58.21
1.5762M	8	4	2	5	58.51
1.5762M		4	0	6	58.51
1.5711	12	7	1	2	58.72
1.5336M	3	-3	1	7	60.30
1.5336M		-3	3	5	60.30
1.5243M	6	-5	1	6	60.71
1.5243M		-2	4	3	60.71
1.5103	4	-4	2	6	61.33

Chromium Sulfate, $Cr_2(SO_4)_3$

CAS registry no.
10101-53-8

Sample
The sample was prepared by heating $NH_4Cr(SO_4)_2$ at 500 °C for 3 hours. The sample contained a very small percent of Cr_2O_3.

Color
Reddish brown

Structure
Hexagonal, $R\bar{3}$ (148), Z = 6. [Kokkoros, 1965].

Lattice constants of this sample
a = 8.132(1) Å
c = 21.943(6)

c/a = 2.6983

Volume
1256.8 Å^3

Density
(calculated) 3.109 g/cm^3

Figure of merit
F_{30} = 40.0(0.014,55)

Reference intensity
$I/I_{corundum}$ = 1.55(5)

Additional patterns
1. PDF card 18-393 [Kokkoros, 1965]
2. PDF card 18-394 [Watelle-Marion and Thiard, 1965]

References

Kokkoros, P. A. (1965). Mineral. Petrogr. Mitt. 10, 45.
Watelle-Marion, G. and Thiard, R. (1965). C. R. Acad. Sci. 261, 4105.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
5.93	50	0 1 2	14.93
4.327	45	1 0 4	20.51
4.070	15	1 1 0	21.82
3.658	25	0 0 6	24.31
3.555	100	1 1 3	25.03
2.965	35	0 2 4	30.11
2.721	40	1 1 6	32.89
2.644	11	2 1 1	33.88
2.395	9	2 1 4	37.52
2.347	11	3 0 0	38.31
2.274	3	1 2 5	39.59
2.235	8	3 0 3	40.32
2.163	9	2 0 8	41.72
2.092	6	1 1 9	43.20
2.029	3	2 1 7	44.61
1.975	4	3 0 6	45.91
1.923	5	3 1 2	47.23
1.909	5	1 2 8	47.59
1.8627	6	0 2 10	48.85
1.8395	4	1 3 4	49.51
1.7771	9	2 2 6	51.37
1.7390	3	0 4 2	52.58
1.6931	11	2 1 10	54.12
1.6573	4	1 3 7	55.39
1.6114	2	3 2 1	57.11
1.5981	3	2 3 2	57.63
1.5903	3	3 1 8	57.94
1.5613	2	2 2 9	59.12
1.5504	6	3 2 4	59.58
1.5366	6	4 1 0	60.17
1.5167	3	2 3 5	61.04
1.4818	3	0 4 8	62.64
1.4586	10	1 3 10	63.75
1.4425	4	3 0 12	64.55

Copper Lead Hydroxide Sulfate, Linarite, $CuPb(OH)_2(SO_4)$

Sample
The hand separated sample is from U.S. National Museum (NMNH R8105) from Mammoth Mine, Pinal Co., AZ.

Major impurities
Approximately 10% $PbSO_4$ was present in this mineral as a second phase and was ignored.

Color
Deep blue

Structure
Monoclinic, $P2_1/m$ (11), Z = 2. The structure was determined by Bachmann and Zeeman [1961]. Araki [1962] re-examined his earlier work and confirmed the above structure.

Lattice constants of this sample
a = 9.6913(9)Å
b = 5.6503(6)
c = 4.6873(5)
β = 102.66(1)°

a/b = 1.7152
c/b = 0.8296

Volume
250.43 Å^3

Density
(calculated) 5.315 g/cm^3

Figure of merit
F_{30} = 76.6(0.011,35)

Additional patterns
1. PDF card 4-598 [Berry, 1951]

References

Araki, T. (1962). Mineral. J. Japan. 3, 282.
Bachmann, H.-G. and Zeeman, J. (1961). Acta Crystallogr. 14, 747.
Berry. L. G. (1951). Amer. Mineral. 36, 512.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
9.46	11	1 0 0	9.34
4.849	40	1 1 0	18.28
4.731	3	2 0 0	18.74
4.521	60	-1 0 1	19.62
3.805	9	1 0 1	23.36
3.717	3	-2 0 1	23.92
3.625	30	2 1 0	24.54
3.556	55	0 1 1	25.02
3.151M	100	1 1 1	28.30
3.151M		3 0 0	28.30
3.106	40	-2 1 1	28.72
2.978	19	2 0 1	29.98
2.912	2	-3 0 1	30.68
2.826	17	0 2 0	31.64
2.754	6	3 1 0	32.49
2.707	30	1 2 0	33.06
2.587	25	-3 1 1	34.64
2.424	8	2 2 0	37.05
2.405	17	0 2 1	37.36
2.365M	5	3 0 1	38.02
2.365M		4 0 0	38.02
2.344	4	-1 0 2	38.37
2.317	20	-4 0 1	38.83
2.267	20	1 2 1	39.72
2.261	20	-2 0 2	39.83
2.250	9	-2 2 1	40.05
2.181M	17	3 1 1	41.36
2.181M		4 1 0	41.36
2.164	19	-1 1 2	41.71
2.145	6	-4 1 1	42.09
2.119M	20	0 1 2	42.63
2.119M		1 0 2	42.63
2.104	12	3 2 0	42.95
2.081	4	-3 0 2	43.45
2.049	8	2 2 1	44.16
2.027	20	-3 2 1	44.67
1.9021M	2	2 0 2	47.78
1.9021M		-5 0 1	47.78
1.8469	5	1 3 0	49.30
1.8295	12	4 1 1	49.80
1.8128M	20	3 2 1	50.29
1.8128M		4 2 0	50.29
1.8018M	17	2 1 2	50.62
1.8018M		-5 1 1	50.62
1.7932	14	5 1 0	50.88
1.7769	7	0 2 2	51.38
1.7660M	9	-4 1 2	51.72
1.7660M		-2 2 2	51.72
1.7497	5	2 3 0	52.24
1.7416	8	0 3 1	52.50

d(Å)	I	hkℓ			2θ(°)
1.6883	5	1	3	1	54.29
1.6803	8	-2	3	1	54.57
1.6752	8	-3	2	2	54.75
1.6456	4	-5	0	2	55.82
1.6264	5	5	0	1	56.54
1.6130	5	3	1	2	57.05
1.5804M	8	-3	3	1	58.34
1.5804M		-5	1	2	58.34
1.5765M	13	-5	2	1	58.50
1.5765M		6	0	0	58.50
1.5718	9	5	2	0	58.69
1.5595	2	-1	0	3	59.20
1.5542M	2	-2	0	3	59.42
1.5542M		-4	2	2	59.42
1.5413	4	-6	1	1	59.97
1.5247	3	0	0	3	60.69
1.5079	4	-3	0	3	61.44
1.5033	4	-1	1	3	61.65
1.4891	6	4	0	2	62.30
1.4736M	4	3	3	1	63.03
1.4736M		4	3	0	63.03
1.4680	4	-1	3	2	63.30
1.4571	2	-3	1	3	63.83
1.4466	2	3	2	2	64.35
1.4216	2	-5	2	2	65.62
1.4124	6	0	4	0	66.10
1.4092+	6	5	2	1	66.27
1.4092+		-6	1	2	66.27
1.3878	2	-4	1	3	67.43
1.3802	3	-7	0	1	67.85
1.3763	4	6	2	0	68.07
1.3655M	3	2	0	3	68.68
1.3655M		-1	2	3	68.68
1.3576	2	6	1	1	69.14
1.3504	5	7	0	0	69.56
1.3490+	6	4	3	1	69.64
1.3490+		-1	4	1	69.64

p-Fluorobenzoic Acid, $C_7H_5FO_2$

CAS registry no.
456-22-4

Sample
The sample was NBS Standard Reference Material 2143.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14), Z = 4. The structure was qualitatively determined by Toussaint [1952].

Lattice constants of this sample
a = 26.545(4) Å
b = 6.385(2)
c = 3.816(1)
β = 93.72(2)°

a/b = 4.1573
c/b = 0.5976

Volume
645.4 Å^3

Density
(calculated) 1.442 g/cm^3

Figure of merit
F_{30} = 60.5(0.012,41)

Reference intensity
$I/I_{corundum}$ = 1.10(4)

Additional pattern
1. PDF card 11-730 [Institute of Physics, Cardiff, Wales]

Reference
Toussaint, J. (1952). Mem. Soc. Roy. Sci. Liege, Collect. 8, 12, 1.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
13.26	85	2 0 0	6.66
6.62	20	4 0 0	13.37
6.21	6	1 1 0	14.26
5.76	20	2 1 0	15.38
5.178	100	3 1 0	17.11
4.600	30	4 1 0	19.28
4.412	2	6 0 0	20.11
4.077	3	5 1 0	21.78
3.805	5	-1 0 1	23.36
3.737	10	1 0 1	23.79
3.580	75	-3 0 1	24.85
3.312	35	8 0 0	26.90
3.274M	70	0 1 1	27.22
3.274M		-1 1 1	27.22
3.226	65	1 1 1	27.63
3.194M	9	0 2 0	27.91
3.194M		-5 0 1	27.91
3.172	7	1 2 0	28.11
3.134	5	2 1 1	28.46
3.005+	4	3 2 0	29.71
3.005+		5 0 1	29.71
2.940	8	8 1 0	30.38
2.875	5	4 2 0	31.08
2.856	4	-5 1 1	31.29
2.715	4	5 1 1	32.97
2.672	5	9 1 0	33.51
2.649	2	10 0 0	33.81
2.586	5	6 2 0	34.66
2.560	3	6 1 1	35.02
2.446+	4	10 1 0	36.71
2.446+		0 2 1	36.71
2.423	5	-2 2 1	37.08
2.404	4	-9 0 1	37.37
2.395	4	-8 1 1	37.52
2.299	7	8 2 0	39.16
2.264M	7	8 1 1	39.79
2.264M		4 2 1	39.79
2.252M	5	11 1 0	40.00
2.252M		-9 1 1	40.00
2.208	1L	12 0 0	40.84
2.164	1	9 2 0	41.70
2.129	2	9 1 1	42.43
2.102M	4	6 2 1	43.00
2.102M		2 3 0	43.00
2.096M	3	-11 0 1	43.12
2.096M		-7 2 1	43.12
2.087	2	12 1 0	43.31
2.039	1	10 2 0	44.40
2.007	1L	-8 2 1	45.15
1.942	1	13 1 0	46.75
1.921M	1	11 2 0	47.28
1.921M		-9 2 1	47.28
1.892	1	14 0 0	48.06
1.847M	3	-2 3 1	49.31
1.847M		-13 0 1	49.31
1.844	3	9 2 1	49.38
1.825	6	0 1 2	49.93
1.815M	2	12 2 0	50.24
1.815M		14 1 0	50.24

CAS registry no.
10294-29-8

Sample
The sample was prepared by dissolving Au metal in aqua regia. The dark red intermediate crystals obtained were dried at 200 °C for one hour. The AuCl crystals were found to be metastable, disproportionately decomposing into Au metal and Au_2Cl_6 [Janssen et al., 1974]. Au_2Cl_6 was not detected in this sample; however, the Au metal present was used as the internal standard.

Color
Yellow

Structure
Tetragonal, $I4_1/amd$ (141), Z = 8. The structure was studied by Janssen et al. [1974]. The structure had been reported to be orthorhombic by Capella and Schwab [1965].

Lattice constants of this sample
a = 6.7425(9) Å
c = 8.694(1)

c/a = 1.2894

Volume
395.2 $Å^3$

Density
(calculated) 7.812 g/cm^3

Figure of merit
F_{16} = 81.8(0.010,20)

Additional patterns
1. PDF card 27-241 [Janssen et al., 1974]
2. Capella and Schwab [1965]

References
Capella, L. and Schwab, C. (1965). C. R. Acad. Sci. 260, 4337.
Janssen, E. M. W., Folmer, J. C. W., and Wiegers, G. A. (1974). J. Less-Common Metals 38, 71.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Au, a = 4.0786 Å

d(Å)	I	hkℓ	2θ(°)
5.327	100	1 0 1	16.63
3.371	4	2 0 0	26.42
3.213	5	1 1 2	27.74
2.849	60	2 1 1	31.37
2.664M	100	2 0 2	33.62
2.664M		1 0 3	33.62
2.384	25	2 2 0	37.71
2.173	18	0 0 4	41.52
2.089	30	2 1 3	43.27
1.8278M	14	3 2 1	49.85
1.8278M		2 0 4	49.85
1.7760	4	3 0 3	51.41
1.6846M	20	4 0 0	54.42
1.6846M		1 0 5	54.42
1.6063M	17	4 1 1	57.31
1.6063M		2 2 4	57.31
1.5711M	10	4 0 2	58.72
1.5711M		3 2 3	58.72
1.5061	4	2 1 5	61.52
1.4245M	20	4 2 2	65.47
1.4245M		4 1 3	65.47
1.3754	4	3 0 5	68.12

Iron Phosphate Hydrate (Vivianite), $Fe_3(PO_4)_2 \cdot 8H_2O$

Sample
The sample was made by slow reaction of H_3PO_4 on $FeSO_4$ solution with some H_2SO_4 added. The flask was freed of air by flushing with natural gas and left with occasional shaking for two weeks.

Color
Grayish purplish blue

Structure
Monoclinic, I2/m (12), Z = 2 [Barth, 1937]. The structure was determined by Mori and Ito [1950]. It is isostructural with $Fe_3(AsO_4)_2 \cdot 8H_2O$ (parasymplesite) [Ritz et al., 1974].

Lattice constants of this sample
a = 10.034(3) Å
b = 13.449(3)
c = 4.707(2)
β = 102.65(3)°

a/b = 0.7461
c/b = 0.3500

Volume
619.7 $Å^3$

Density
(calculated) 2.688 g/cm^3

Figure of merit
F_{30} = 52.6 (0.015,38)

Polymorphism
A polymorph of $Fe_3(PO_4)_2 \cdot 8H_2O$ occurs naturally, is triclinic and is called metavivianite [Ritz et al., 1974].

Additional pattern
1. PDF card 3-70 [Dow Chemical Co., Midland, MI]

References
Barth, T. F. W. (1937). Amer. Mineral. 22, 325.
Mori, H. and Ito, T. (1950). Acta Crystallogr. 3, 1.
Ritz, C., Essene, E. J., and Peacor, D. R. (1974). Amer. Mineral. 59, 896.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
7.93	13	1 1 0	11.15
6.73	100	0 2 0	13.15
4.900	12	2 0 0	18.09
4.558	5	-1 0 1	19.46
4.341	2	0 1 1	20.44
4.081	12	1 3 0	21.76
3.849	7	1 0 1	23.09
3.768	1L	-1 2 1	23.59
3.361	1	0 4 0	26.50
3.343	2	1 2 1	26.64
3.210	16	0 3 1	27.77
2.985	10	-3 0 1	29.91
2.960	8	2 1 1	30.17
2.770	4	2 4 0	32.29
2.728	9	-3 2 1	32.80
2.706	9	-1 4 1	33.08
2.637	6	3 3 0	33.97
2.593	4	1 5 0	34.57
2.530	8	1 4 1	35.45
2.514	3	2 3 1	35.68
2.448	1	4 0 0	36.68
2.421	6	3 0 1	37.11
2.321	7	0 5 1	38.77
2.296	1	0 0 2	39.20
2.279M	1	-2 0 2	39.51
2.279M		3 2 1	39.51
2.233	5	-3 4 1	40.35
2.194	5	-2 5 1	41.11
2.173	2	0 2 2	41.53
2.108M	1	1 1 2	42.86
2.108M		-4 3 1	42.86
2.075	4	3 5 0	43.59
2.039	1L	2 6 0	44.40
2.012M	2	2 5 1	45.03
2.012M		-1 6 1	45.03
1.964M	2	3 4 1	46.19
1.964M		-5 0 1	46.19
1.936M	2	5 1 0	46.89
1.936M		1 6 1	46.89
1.886M	2	1 7 0	48.22
1.886M		-5 2 1	48.22
1.816	2	4 3 1	50.20
1.793	1	-3 6 1	50.89
1.786	3	-4 5 1	51.10
1.772	2	0 7 1	51.52
1.6809	6	0 8 0	54.55
1.6599	2	-3 5 2	55.30
1.5974M	3	4 5 1	57.66
1.5974M		3 3 2	57.66
1.5834	4	5 5 0	58.22
1.5404	1	1 8 1	60.01

Iron Sulfate, $Fe_2(SO_4)_3$

CAS registry no.
10028-22-5

Sample
The sample was made by heating $Fe_2(SO_4)_3 \cdot XH_2O$ at 200 °C for several hours, followed by heating at 500 °C in a sealed glass tube for 1 hour.

Color
Yellow white

Structure
Hexagonal, $R\bar{3}$ (148), Z = 6 [Kokkoros, 1965].

Lattice constants of this sample
a = 8.236(1) Å
c = 22.166(6)

c/a = 2.6914

Volume
1302.1 $Å^3$

Density
(calculated) 3.060 g/cm^3

Figure of Merit
F_{30} = 32.8(0.017,53)

Reference intensity
$I/I_{corundum}$ = 2.26(11)

Additional pattern
1. PDF card 18-652 [Kokkoros, 1965]

Reference
Kokkoros, P. A. (1965). Tschermak's Mineral. Petrogr. Mitt. 10, 45.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
6.01	50	0 1 2	14.72
4.380	45	1 0 4	20.26
4.124	13	1 1 0	21.53
3.699	7	0 0 6	24.04
3.599	100	1 1 3	24.72
3.002	40	0 2 4	29.74
2.751	45	1 1 6	32.52
2.678	10	2 1 1	33.43
2.581	1	0 1 8	34.73
2.426	9	2 1 4	37.03
2.378	12	3 0 0	37.80
2.301	1	1 2 5	39.11
2.263	7	3 0 3	39.80
2.190	2	2 0 8	41.19
2.114	7	1 1 9	42.74
2.054	3	2 1 7	44.06
1.999	4	3 0 6	45.33
1.947	3	3 1 2	46.62
1.931	4	1 2 8	47.01
1.882	6	0 2 10	48.31
1.863	6	1 3 4	48.85
1.847	1	0 0 12	49.31
1.799	11	2 2 6	50.71
1.760	3	0 4 2	51.90
1.7123	11	2 1 10	53.47
1.6781	4	1 3 7	54.65
1.6330	1	3 2 1	56.29
1.6099	5	3 1 8	57.17
1.5794	1	2 2 9	58.38
1.5694	7	3 2 4	58.79
1.5561	7	4 1 0	59.34
1.5346	2	2 3 5	60.26
1.5231	2	4 1 3	60.76
1.4995	2	0 4 8	61.82
1.4757	7	1 3 10	62.93

Lead Bromide Hydroxide, PbBr(OH)

CAS registry no.
16651-91-5

Sample
The sample was prepared by making a saturated aqueous solution of fresh recrystallized $PbBr_2$. To this was added a 10% solution of NaOH. The precipitate was left for 80 hours in the liquid to promote growth of the crystals.

Color
Colorless

Structure
Orthorhombic, Pnam (62), Z = 4. The structure of PbBr(OH) was determined by Møller [1966]. PbBr(OH) is isostructural with SbBrS and PbCl(OH).

Lattice constants of this sample
a = 7.3850(8)Å
b = 10.013(1)
c = 4.0835(5)

a/b = 0.7375
c/b = 0.4078

Volume
301.96 $Å^3$

Density
(calculated) 6.689 g/cm^3

Figure of merit
F_{30} = 78.7(0.012,31)

Reference Intensity
$I/I_{corundum}$ = 5.9(3)

Additional patterns
1. PDF card 6-257 [Shell Petroleum Co., Ltd.]
2. Møller [1966]

Reference
Møller, C. K. (1966). Kgl. Dan. Vidensk. Sels. Mat. Fys. Medd. 35, 15.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
5.93	9	1 1 0	14.93
4.998	9	0 2 0	17.73
4.139	55	1 2 0	21.45
3.781	4	0 1 1	23.51
3.693	10	2 0 0	24.08
3.462	25	2 1 0	25.71
3.363	100	1 1 1	26.48
3.042	12	1 3 0	29.34
2.970	20	2 2 0	30.06
2.908	45	1 2 1	30.72
2.737	4	2 0 1	32.69
2.641	40	2 1 1	33.91
2.584	50	0 3 1	34.69
2.504	6	0 4 0	35.83
2.475	10	2 3 0	36.26
2.439	3	1 3 1	36.82
2.403	18	2 2 1	37.40
2.391	25	3 1 0	37.59
2.371	20	1 4 0	37.92
2.210	15	3 2 0	40.80
2.118	19	2 3 1	42.65
2.072	4	2 4 0	43.64
2.064	6	3 1 1	43.83
2.043	20	0 0 2	44.31
1.982	2	3 3 0	45.75
1.943	14	3 2 1	46.70
1.933	8	1 5 0	46.97
1.8901	2	0 2 2	48.10
1.8483	4	2 4 1	49.26
1.8313	12	1 2 2	49.75
1.7975	8	0 5 1	50.75
1.7860	6	2 0 2	51.10
1.7824	5	3 3 1	51.21
1.7597M	7	2 5 0	51.92
1.7597M		2 1 2	51.92
1.7475	13	1 5 1	52.31
1.6959	4	1 3 2	54.03
1.6823M	25	2 2 2	54.50
1.6823M		4 0 1	54.50
1.6688	3	0 6 0	54.98
1.6151	19	4 3 0	56.97
1.6120	20	3 4 1	57.09
1.5944	2	4 2 1	57.78
1.5824	4	0 4 2	58.26
1.5757	5	2 3 2	58.53
1.5531M	16	3 5 0	59.47
1.5531M		3 1 2	59.47
1.5476	14	1 4 2	59.70
1.5211	7	2 6 0	60.85
1.5123	1	1 6 1	61.24

d(Å)	I	hkℓ			2θ(°)
1.4998	7	3	2	2	61.81
1.4610	4	5	1	0	63.64
1.4518	7	3	5	1	64.09
1.4251	7	2	6	1	65.44
1.4166	3	5	2	0	65.88
1.4036M	4	1	7	0	66.57
1.4036M		1	5	2	66.57
1.3967	3	4	4	1	66.94
1.3811	1	3	6	0	67.80
1.3692	1	4	0	2	68.47
1.3574M	2	4	5	0	69.15
1.3574M		4	1	2	69.15
1.3499	3	0	7	1	69.59
1.3385	5	5	2	1	70.27
1.3276	9	1	7	1	70.93
1.2929	4	1	2	3	73.14
1.2820	2	5	3	1	73.86
1.2669M	10	4	3	2	74.89
1.2669M		2	1	3	74.89
1.2603	6	0	3	3	75.35
1.2513	1	0	8	0	75.99
1.2426	1	1	3	3	76.62
1.2197	6	2	6	2	78.33
1.2146	5	5	4	1	78.72
1.1928	3	2	3	3	80.45
1.1885M	5	5	5	0	80.80
1.1885M		5	1	2	80.80

Lithium Calcium Aluminum Boron Hydroxy Silicate, Liddicoatite, $Ca(Li,Al)_3Al_6B_3Si_6O_{27}(O,OH)_3(OH,F)$

Sample
The sample is holotype material from U.S. National Museum (NMNH #135815). The locality of this sample can be stated only in general terms. The crystals occur as detritus in the soils near Antsirabe in Madagascar, and a specific site for the occurrence of the type mineral is not known [Dunn et al., 1977].

Color
Dark olive brown

Optical data
Uniaxial(-), N_o = 1.637, N_e = 1.621 [Dunn et al., 1977].

Structure
Hexagonal, R3m (160), Z = 3, isostructural with tourmalines [Dunn et al., 1977].

Lattice constants of this sample
a = 15.847(1) Å
c = 7.1080(7)

c/a = 0.4485

Volume
1546.0 $Å^3$

Density
(calculated) 3.06 g/cm^3 [based on $Ca(Li_{1.74}Al_{1.26})Al_6B_3Si_6O_{27.52}(OH)_{2.48}(F,OH)$ according to empirical formula by Dunn et al. (1977)].

Figure of merit
F_{30} = 62.0(0.015,32)

Reference
Dunn, P. J., Appleman, D. E., and Nelen, J. E. (1977). Amer. Mineral. 62, 1121.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
7.94	5	1 1 0	11.14
6.33	6	1 0 1	13.99
4.943	30	0 2 1	17.93
4.581	19	3 0 0	19.36
4.197	50	2 1 1	21.15
3.962	55	2 2 0	22.42
3.445	50	0 1 2	25.84
3.357	25	1 3 1	26.53
3.093	9	4 0 1	28.84
2.995	30	4 1 0	29.81
2.933	100	1 2 2	30.45
2.881	9	3 2 1	31.02
2.641	2	3 3 0	33.92
2.598	14	3 1 2	34.49
2.559	85	0 5 1	35.04
2.468	1	0 4 2	36.37
2.437	4	2 4 1	36.85
2.368	18	0 0 3	37.96
2.356	15	2 3 2	38.17
2.328	24	5 1 1	38.65
2.288	5	6 0 0	39.34
2.270	4	1 1 3	39.67
2.173	7	5 0 2	41.53
2.151	17	4 3 1	41.96
2.105	19	3 0 3	42.94
2.095	19	4 2 2	43.15
2.033	30	2 2 3	44.53
2.025	40	1 5 2	44.71
2.008	6	1 6 1	45.12
1.980	5	4 4 0	45.78
1.9054	35	3 4 2	47.69
1.8901	3	3 5 1	48.10
1.8582	5	4 1 3	48.98
1.8375	7	6 2 1	49.57
1.8031	3	6 1 2	50.58
1.7619	10	1 0 4	51.85
1.7200	1	0 2 4	53.21
1.7061	2	5 4 1	53.68
1.6812	2	2 1 4	54.54
1.6781	3	2 6 2	54.65
1.6459	17	6 0 3	55.81
1.6319	14	2 7 1	56.33
1.6112	2	5 2 3	57.12
1.5851	13	5 5 0	58.15
1.5782	8	4 0 4	58.43
1.5750	6	4 5 2	58.56
1.5670	3	8 1 1	58.89
1.5479	3	3 2 4	59.69
1.5371	4	4 6 1	60.15
1.5247	6	9 0 0	60.69

d(Å)	I	hkℓ	2θ(°)
1.5161	6	7 2 2	61.07
1.4974	4	8 2 0	61.92
1.4913	14	0 5 4	62.20
1.4655	6	2 4 4	63.42
1.4414	20	5 1 4	64.61
1.4226	3	7 4 0	65.57
1.4139	5	0 1 5	66.02
1.4102	7	1 9 1	66.22
1.3958M	17	6 3 3	66.99
1.3958M		4 3 4	66.99
1.3713	1	1 2 5	68.35
1.3475	8	10 0 1	69.73
1.3334	2	5 6 2	70.58
1.3208	4	6 6 0	71.35
1.3167M	8	5 5 3	71.61
1.3167M		3 5 4	71.61
1.3134	8	0 4 5	71.82
1.3022	10	10 1 0	72.53
1.2987	7	6 2 4	72.76
1.2926	2	5 7 1	73.16
1.2826	2	9 0 3	73.82
1.2760	2	8 4 1	74.27
1.2690	4	9 3 0	74.75
1.2656	5	8 2 3	74.98
1.2622	12	5 0 5	75.22
1.2496	5	5 4 4	76.11
1.2463	3	4 2 5	76.35
1.2316	3	1 5 5	77.43
1.2316	3	1 5 5	77.43
1.2289	4	0 11 1	77.63

Lithium Chromium Oxide Hydrate, $Li_2CrO_4 \cdot 2H_2O$

Sample
The sample was made by slow evaporation at room temperature of an aqueous solution of Li_2CrO_4.

Color
Strong orange yellow

Structure
Orthorhombic, $P2_12_12_1$ (19), Z = 4. The cell was obtained from the axial ratios of Groth [1908] assuming a density near 2.1 and a Z = 4.

Lattice constants of this sample
a = 7.746(1) Å
b = 12.011(2)
c = 5.5094(7)

a/b = 0.6449
c/b = 0.4587

Volume
512.56 Å^3

Density
(calculated) 2.150 g/cm^3

Figure of merit
F_{30} = 74.6(0.012,35)

Additional pattern
1. PDF card 1-819 [Hanawalt et al., 1938]

Reference
Groth, P. (1908). Chemische Krystallographie II, (Wilhelm Engelmann, Leipzig, Germany) p. 365.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

CuK$\alpha_1\lambda$ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
6.52	25	1 1 0	13.57
5.012	25	0 1 1	17.68
4.751	90	1 2 0	18.66
4.489	85	1 0 1	19.76
4.205	75	1 1 1	21.11
4.061	85	0 2 1	21.87
3.687	60	2 1 0	24.12
3.593	25	1 2 1	24.76
3.558	60	1 3 0	25.01
3.239	4	0 3 1	27.52
3.170	70	2 0 1	28.13
3.062	100	2 1 1	29.14
3.002	75	0 4 0	29.74
2.993	75	1 3 1	29.83
2.802M	11	2 2 1	31.91
2.802M		1 4 0	31.91
2.784	20	2 3 0	32.13
2.754	80	0 0 2	32.48
2.685	12	0 1 2	33.34
2.597	3	1 0 2	34.51
2.537	7	1 1 2	35.35
2.525	7	3 1 0	35.52
2.494	25	1 4 1	35.98
2.485	45	2 3 1	36.12
2.382	19	1 2 2	37.74
2.373M	40	2 4 0	37.89
2.373M		3 2 0	37.89
2.338	25	3 0 1	38.48
2.293M	5	1 5 0	39.25
2.293M		3 1 1	39.25
2.271	3	0 3 2	39.66
2.245	4	2 0 2	40.14
2.206	14	2 1 2	40.88
2.179M	45	2 4 1	41.40
2.179M		3 2 1	41.40
2.170	17	3 3 0	41.59
2.118	12	1 5 1	42.65
2.103	13	2 2 2	42.98
2.041	16	2 5 0	44.34
2.029	10	0 4 2	44.62
2.018	11	3 3 1	44.87
1.9586M	5	2 3 2	46.32
1.9586M		3 4 0	46.32
1.9365	8	4 0 0	46.88
1.9134	20	2 5 1	47.48
1.8839	9	3 0 2	48.27
1.8614	5	3 1 2	48.89
1.8424	4	4 2 0	49.43
1.8271M	4	4 0 1	49.87
1.8271M		1 6 1	49.87
1.8149	12	0 1 3	50.23
1.8061	10	4 1 1	50.49
1.7988	5	2 4 2	50.71
1.7863	7	1 0 3	51.09
1.7676	9	1 1 3	51.67
1.7481	2	4 2 1	52.29
1.7135	1	1 2 3	53.43
1.6755M	9	3 5 1	54.74
1.6755M		1 7 0	54.74
1.6591	25	2 0 3	55.33
1.6435	6	2 1 3	55.90
1.6272	20	4 4 0	56.51
1.6030	3	1 7 1	57.44
1.5962	7	3 4 2	57.71
1.5824	3	3 6 0	58.26
1.5708	4	4 1 2	58.73

Lithium Tin Oxide, Li_2SnO_3

CAS registry no.
12188-25-9

Sample
The sample was prepared by heating $Li_2C_2O_4$ and SnO_2 at 800 °C for 10 minutes followed by 950 °C for 20 minutes.

Color
Colorless

Structure
Monoclinic, A2/a (15), Z = 8, [Scheer et al., 1955; Lang, 1954]. The structure of Li_2SnO_3 has been studied by Kreuzburg et al. [1970].

Lattice constants of this sample
a = 10.027(2) Å
b = 9.181(2)
c = 5.301(2)
β = 100.26(2)°

a/b = 1.0921
c/b = 0.5774

Volume
480.1 Å^3

Density
(calculated) 4.996 g/cm^3

Figure of merit
F_{30} = 27.9(0.014,80)

Reference intensity
$I/I_{corundum}$ = 4.1(3)

Polymorphism
There is a second form of Li_2SnO_3 which differs in its stacking [Lang, 1966].

References

Kreuzburg, G., Stewner, F., and Hoppe, R. (1970). Z. Anorg. Allg. Chem. 379, 242.
Lang, G. (1954). Z. Anorg. Allg. Chem. 276, 77.
Lang, G. (1966). Z. Anorg. Allg. Chem. 348, 246.
Scheer, J. J., Van Arkel, A. E., and Heyding, R. D. (1955). Can. J. Chem. 33, 683.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
4.932	100	2 0 0	17.97
4.586	17	0 2 0	19.34
4.539	10	0 1 1	19.54
4.386	7	-1 1 1	20.23
4.166	3	1 2 0	21.31
3.899	2	1 1 1	22.79
3.630	2	-2 1 1	24.50
3.106	1	2 1 1	28.72
2.886	1	-3 1 1	30.96
2.673	2	3 2 0	33.50
2.641	1	0 3 1	33.92
2.608M	55	-1 3 1	34.36
2.608M		0 0 2	34.36
2.495M	25	-2 0 2	35.97
2.495M		1 3 1	35.97
2.466	9	4 0 0	36.40
2.324	1	-4 1 1	38.72
2.293	3	0 4 0	39.25
2.288	2	-1 2 2	39.34
2.154M	65	-3 3 1	41.91
2.154M		2 0 2	41.91
1.974	20	3 3 1	45.94
1.7343	3	-1 1 3	52.74
1.7321M	3	-1 4 2	52.81
1.7321M		0 5 1	52.81
1.7233M	2	-1 5 1	53.10
1.7233M		0 4 2	53.10
1.6527	12	-5 3 1	55.56
1.6446	6	6 0 0	55.86
1.6180	1	-5 2 2	56.86
1.5300M	19	0 6 0	60.46
1.5300M		-1 3 3	60.46
1.5164	17	5 3 1	61.06
1.4612M	15	2 6 0	63.63
1.4612M		1 3 3	63.63
1.3202M	6	-2 0 4	71.39
1.3202M		0 6 2	71.39
1.3041M	5	-6 1 3	72.41
1.3041M		0 0 4	72.41
1.3002	7	4 6 0	72.66
1.2921	3	-7 3 1	73.19
1.2723M	2	0 7 1	74.52
1.2723M		-1 2 4	74.52
1.2685M	1	-2 2 4	74.78
1.2685M		-1 7 1	74.78
1.2473	9	2 6 2	76.28
1.2325	3	1 5 3	77.36
1.2093	3	5 6 0	79.13
1.2081M	3	2 0 4	79.23
1.2081M		4 3 3	79.23
1.1990	4	7 3 1	79.95
1.1459M	1L	8 1 1	84.48
1.1459M		-5 6 2	84.48
1.1224	4	4 6 2	86.68

Magnesium Sulfate Hydrate (Kieserite), $MgSO_4 \cdot H_2O$

CAS registry no.
14567-64-7

Sample
A sample of $MgSO_4 \cdot 7H_2O$ was obtained from Fisher Scientific Co. of Fairlawn, NJ. The material was heated first at 150 °C, then sealed in a tube and heated for 1 3/4 hours at 400 °C.

Color
Colorless

Structure
Monoclinic, A2/a (15), Z = 4. The structure was determined by Leonhardt and Weiss [1957] and confirmed by Bregeault et al. [1972].

Lattice constants of this sample
a = 7.5110(9) Å
b = 7.611(1)
c = 6.921(1)
β = 116.17(1)°

a/b = 0.9868
c/b = 0.9093

Volume
355.1 $Å^3$

Density
(calculated) 2.589 g/cm^3

Figure of merit
F_{30} = 60.5(0.011,47)

Reference intensity
$I/I_{corundum}$ = 1.02(4)

Additional pattern
1. PDF card 13-102 [Kubisz, 1960] (natural mineral)

References
Bregeault, J.-M., Herpin, P., and Coing-Boyat, J. (1972). Bull. Soc. Chim. Fr. 1972, 2247.
Kubisz, J. (1960). Bull. Acad. Pol. Sci. Ser. Sci. Geol. Geogr. 8, 101.
Leonhardt, H. J. and Weiss, R. (1957). Naturwissenschaften 44, 338.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
4.815	75	0 1 1	18.41
3.405	100	1 1 1	26.15
3.351	70	-2 1 1	26.58
3.313	70	1 2 0	26.89
3.106	13	0 0 2	28.72
3.051	40	-2 0 2	29.25
2.560	35	-1 2 2	35.03
2.523	30	2 2 0	35.55
2.401	3	2 1 1	37.42
2.380	3	-2 2 2	37.76
2.342	4	-1 3 1	38.41
2.185	7	-1 1 3	41.28
2.099	9	-2 3 1	43.07
2.054	20	1 2 2	44.05
2.023	3	-3 2 2	44.77
1.965	8	-3 1 3	46.16
1.934	4	3 2 0	46.94
1.9039M	5	2 0 2	47.73
1.9039M		0 4 0	47.73
1.8657	1	-4 0 2	48.77
1.8125	3	3 1 1	50.30
1.7919M	1	-4 1 1	50.92
1.7919M		2 3 1	50.92
1.7288M	1L	-2 0 4	52.92
1.7288M		1 1 3	52.92
1.7029	3	2 2 2	53.79
1.6750	14	-4 2 2	54.76
1.6577	5	2 4 0	55.38
1.6227	8	0 4 2	56.68
1.6043	3	0 3 3	57.39
1.5866	7	-3 3 3	58.09
1.5531	4	0 0 4	59.47
1.5401M	2	4 2 0	60.02
1.5401M		-1 2 4	60.02
1.5265	2	-3 2 4	60.61
1.5030	4	3 3 1	61.66
1.4524M	3	1 3 3	64.06
1.4524M		3 4 0	64.06
1.4366	2	-5 1 3	64.85
1.4160	2	-4 2 4	65.91
1.3975	1	-5 2 2	66.90

Manganese Phosphate, $Mn_3(PO_4)_2$

Sample
The sample was prepared by heating a 3:2 molar mixture of $MnCO_3$ and $(NH_4)_2HPO_4$ overnight at 850 °C.

Color
Pinkish white

Structure
Monoclinic, $P2_1/c$ (14), Z = 4. The cell was found by use of the Visser program [1969] and by comparison with β-$Zn_3(PO_4)_2$ and $Cd_3(PO_4)_2$. The space group was assigned by consideration of the absences in the powder pattern.

Lattice constants of this sample
a = 8.446(2) Å
b = 10.059(3)
c = 8.047(2)
β = 114.27(2)°

a/b = 0.8396
c/b = 0.8000

Volume
623.2 $Å^3$

Density
(calculated) 3.781 g/cm^3 (assuming Z = 4)

Figures of merit
F_{30} = 54.0(0.013,44)
M_{20} = 31.1

Polymorphism
$Mn_3(PO_4)_2$ is also reported to crystallize in a graftonite structure [Calvo, 1968]. Stephens and Calvo [1969] also describe a second monoclinic form of $Mn_3(PO_4)_2$ which they call "β".

Additional pattern
1. PDF card 3-0465 [Dow Chemical Co., Midland, MI]

References
Calvo, C. (1968). Amer. Mineral. 53, 742.
Stephens, J. S. and Calvo, C. (1969). Can. Chem. 47, 2215.
Visser, J. W. (1969). J. Appl. Crystallogr. 2, 89.

CuK_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.10	8	1 1 0	14.50
5.92	6	0 1 1	14.96
4.207	35	1 2 0	21.10
4.010	16	-1 0 2	22.15
3.852	7	2 0 0	23.07
3.726	55	-1 1 2	23.86
3.669	10	0 0 2	24.24
3.597	12	2 1 0	24.73
3.458	25	-2 0 2	25.74
3.446	13	0 1 2	25.83
3.341	35	1 2 1	26.66
3.269	90	-2 1 2	27.26
3.218	100	-2 2 1	27.70
3.135	30	-1 2 2	28.45
3.073	65	1 3 0	29.03
3.018	25	-1 3 1	29.58
2.963	45	0 2 2	30.14
2.882	60	1 0 2	31.01
2.849	20	-2 2 2	31.37
2.827	55	2 1 1	31.62
2.772	10	1 1 2	32.27
2.705	9	-3 1 1	33.09
2.681M	4	1 3 1	33.40
2.681M		-3 0 2	33.40
2.616	9	-2 3 1	34.25
2.593	25	-3 1 2	34.57
2.573	25	-1 3 2	34.84
2.528	60	2 3 0	35.48
2.489	2	3 1 0	36.06
2.453	14	-3 2 1	36.60
2.408	8	-2 3 2	37.31
2.375	20	0 1 3	37.85
2.368	18	-3 2 2	37.97
2.357	18	-1 2 3	38.15
2.315	9	-2 2 3	38.87
2.285	2	3 2 0	39.41
2.248	4	-3 1 3	40.08
2.215	5	2 3 1	40.71
2.184M	5	2 1 2	41.30
2.184M		1 3 2	41.30
2.157	6	-2 4 1	41.85
2.132	3	-1 4 2	42.37
2.095+	5	-4 0 2	43.15
2.095+		-3 3 2	43.15
2.089	8	-1 3 3	43.28
2.052M	15	-4 1 2	44.09
2.052M		1 1 3	44.09
2.034	11	-2 4 2	44.50
2.006	2	-2 0 4	45.16
1.986	2	3 2 1	45.64

Manganese Phosphate, $Mn_3(PO_4)_2$ - (continued)

d(Å)	I	hkℓ			2θ(°)
1.975M	7	0	3	3	45.92
1.975M		-1	0	4	45.92
1.968	11	-2	1	4	46.08
1.940M	13	-1	1	4	46.80
1.940M		0	5	1	46.80
1.933+	17	1	2	3	46.96
1.933+		-4	2	2	46.96
1.916	20	-4	1	3	47.40
1.891	6	4	1	0	48.09
1.874M	8	-3	4	1	48.53
1.874M		-3	1	4	48.53
1.860	16	2	3	2	48.93
1.835M	9	-3	4	2	49.64
1.835M		1	5	1	49.64

Manganese Sulfate Hydrate (Szmikite), $MnSO_4 \cdot H_2O$

Sample
A sample of $MnSO_4$ was obtained from J. T. Baker Co., Phillipsburg, NJ. Crystals were formed from a saturated solution of the material at room temperature. The crystals slowly changed to the monohydrate when left in open air and were finally heated at 250 °C for 2½ hours.

Color
Colorless

Structure
Monoclinic, A2/a (15), Z = 4, isostructural with $CoSO_4 \cdot H_2O$. The structure was determined by Le Fur et al. [1966].

Lattice constants of this sample
a = 7.766(1) Å
b = 7.666(1)
c = 7.120(1)
β = 115.85(1)°

a/b = 1.0130
c/b = 0.9288

Volume
381.5 Å^3

Density
(calculated) 2.943 g/cm^3

Figure of merit
F_{30} = 77.8(0.010,37)

Reference intensity
$I/I_{corundum}$ = 1.91(7)

Additional pattern
1. PDF card 14-166 [Pistorius, 1961]

References

Le Fur, Y., Coing-Boyat, J., and Bassi, G. (1966). C. R. Acad. Sci. Ser. C 262, 632.
Pistorius, C. W. F. T. (1961). Z. Anorg. Allg. Chem. 302, 226.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
4.916	50	0 1 1	18.03
4.855	30	-1 1 1	18.26
3.834	8	0 2 0	23.18
3.507	100	1 1 1	25.38
3.445	20	-2 1 1	25.84
3.361	30	1 2 0	26.50
3.203	1L	0 0 2	27.83
3.139	40	-2 0 2	28.41
2.606	15	-1 2 2	34.38
2.580	30	2 2 0	34.74
2.483	1	2 1 1	36.15
2.457	1	0 2 2	36.54
2.446	3	-3 1 1	36.71
2.366	7	-1 3 1	38.00
2.245	10	-1 1 3	40.13
2.145	6	1 3 1	42.09
2.131	2	-2 3 1	42.38
2.109	7	1 2 2	42.85
2.072	1	-3 2 2	43.65
2.0193	8	-3 1 3	44.85
1.9894	1	3 2 0	45.56
1.9722	4	2 0 2	45.98
1.9164	2	0 4 0	47.40
1.8762	4	3 1 1	48.48
1.8536	1L	-4 1 1	49.11
1.8316	1L	2 3 1	49.74
1.8159	1L	-3 3 1	50.20
1.7795	1	-2 0 4	51.30
1.7528	4	2 2 2	52.14
1.7472	2	4 0 0	52.32
1.7291	2	-1 3 3	52.91
1.7218M	8	-4 2 2	53.15
1.7218M		-2 3 3	53.15
1.6806	3	2 4 0	54.56
1.6443	5	0 4 2	55.87
1.6389	3	0 3 3	56.07
1.6193	5	-3 3 3	56.81
1.6149	4	-2 2 4	56.98
1.6015	3	0 0 4	57.50
1.5896	1L	4 2 0	57.97
1.5809	1	-1 2 4	58.32
1.5701	1	-4 0 4	58.76
1.5658	1L	-3 2 4	58.94
1.5432	3	3 3 1	59.89
1.5128	1L	-3 4 2	61.22
1.4961	1L	4 1 1	61.98
1.4887M	2	-1 5 1	62.32
1.4887M		1 3 3	62.32
1.4810M	3	-5 1 1	62.68
1.4810M		-5 1 3	62.68
1.4778	2	0 2 4	62.83
1.4643M	1L	-4 3 3	63.48
1.4643M		3 2 2	63.48
1.4526	1L	-4 2 4	64.05
1.4390	1L	-5 2 2	64.73
1.4290	1L	1 5 1	65.24

Mercury Sulfate, $HgSO_4$

Sample
The sample was obtained from Alfa Division, Ventron Corp., Danvers, MA.

Color
Yellowish white

Structure
Orthorhombic, $P2_1mn$ (31), Z = 2. The structure was determined by Bonefačić [1963] and Kokkoros and Rentzeperis [1963]. Aurivillius [1964] reports that the symmetry is monoclinic rather than orthorhombic.

Lattice constants of this sample
a = 4.8150(2) Å
b = 6.5752(3)
c = 4.7810(2)

a/b = 0.7323
c/b = 0.7271

Volume
151.36 Å^3

Density
(calculated) 6.509 g/cm^3

Figure of merit
F_{30} = 118(0.008,31)

Additional patterns
1. PDF card 13-519 [Kokkoros and Rentzeperis, U. Thessaloniki, Greece]
2. Aurivillius and Malmros [1961]

References

Aurivillius, K. (1964). Ark. Kemi 24, 151.
Aurivillius, K. and Malmros, B. (1961). Acta Chem. Scand. 15, 1932.
Bonefačić, A. (1963). Croat. Chem. Acta 35, 195.
Kokkoros, P. A. and Rentzeperis, P. J. (1963). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 119, 234.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
4.782	12	0 0 1	18.54
3.884	85	1 1 0	22.88
3.865	85	0 1 1	22.99
3.392	100	1 0 1	26.25
3.288	75	0 2 0	27.10
3.014	45	1 1 1	29.62
2.707	4	0 2 1	33.06
2.408	25	2 0 0	37.32
2.390	17	0 0 2	37.60
2.361	60	1 2 1	38.09
2.2457	20	0 1 2	40.12
2.1509	10	2 0 1	41.97
2.1412	20	1 0 2	42.17
2.0431	35	2 1 1	44.30
2.0361	25	1 1 2	44.46
1.9936M	35	1 3 0	45.46
1.9936M		0 3 1	45.46
1.9423	25	2 2 0	46.73
1.9333	16	0 2 2	46.96
1.8406	12	1 3 1	49.48
1.7988	8	2 2 1	50.71
1.7939	14	1 2 2	50.86
1.6967	7	2 0 2	54.00
1.6440	17	0 4 0	55.88
1.6154	7	0 3 2	56.96
1.5936	3	0 0 3	57.81
1.5593	5	3 1 0	59.21
1.5545	4	0 4 1	59.41
1.5353	9	2 3 1	60.23
1.5313	8	1 3 2	60.40
1.5215	6	3 0 1	60.83
1.5128	1L	1 0 3	61.22
1.5077	5	2 2 2	61.45
1.4791	15	1 4 1	62.77
1.4743	19	1 1 3	63.00
1.4342	3	0 2 3	64.97
1.3807	10	3 2 1	67.82
1.3576	5	2 4 0	69.14
1.3541	5	0 4 2	69.34
1.3415	5	2 3 2	70.09
1.3329	1	3 0 2	70.61
1.3293	3	2 0 3	70.83
1.3060M	4	3 1 2	72.29
1.3060M		2 4 1	72.29
1.3039	5	1 4 2	72.42
1.2950	1	3 3 0	73.00
1.2684M	4	1 5 0	74.79
1.2684M		0 5 1	74.79
1.2502	1	3 3 1	76.07
1.2452	5	1 3 3	76.43

Mercury Sulfate, $HgSO_4$ - (continued)

d(Å)	I	hkℓ	2θ(°)
1.2348	2	3 2 2	77.19
1.2320	4	2 2 3	77.40
1.2261	2	1 5 1	77.84
1.2035	1	4 0 0	79.59
1.1804	2	2 4 2	81.47
1.1758	3	0 1 4	81.86
1.1673	1L	4 0 1	82.58
1.1601	2	1 0 4	83.21
1.1522	2	0 5 2	83.91
1.1442	1	0 4 3	84.63
1.1387	1	3 3 2	85.14
1.1302	1	4 2 0	85.93
1.1218	2	2 5 1	86.73
1.1206	1	1 5 2	86.85
1.1166	4	3 4 1	87.24
1.1144	4	3 1 3	87.45
1.1002	1L	4 2 1	88.88
1.0960	2	0 6 0	89.31
1.0940	2	1 2 4	89.52
1.0751	1L	4 0 2	91.53
1.0681	1L	0 6 1	92.30
1.0611	1	4 1 2	93.09
1.0566	2	2 1 4	93.61
1.0493	2	0 3 4	94.46
1.0430	3	1 6 1	95.22
1.0394	3	2 5 2	95.65
1.0352	1	3 4 2	96.16
1.0335	2	2 4 3	96.37
1.0302	1	4 3 1	96.78
1.0254	1L	1 3 4	97.39
1.0218	2	4 2 2	97.85
1.0171	1L	3 5 0	98.46
1.0050	3	3 3 3	100.08
.9974	2	2 6 0	101.13
.9949	2	3 5 1	101.47
.9924	3	1 5 3	101.83

Mercury Sulfate, Hg_2SO_4

Sample
The sample was reagent material obtained from Kahlbaum, Berlin, Germany.

Color
Yellowish white

Structure
Monoclinic, P2/a (13), Z = 2, isostructural with mercury selenate. The structure was determined by Dorm [1969].

Lattice constants of this sample
a = 8.365(1) Å
b = 4.4262(5)
c = 6.2785(9)
β = 91.77(1)°

a/b = 1.8899
c/b = 1.4185

Volume
232.34 Å^3

Density
(calculated) 7.108 g/cm^3

Figure of merit
F_{30} = 76.4(0.013,30)

Reference intensity
$I/I_{corundum}$ = 3.4(3)

Additional pattern
1. PDF card 1-0838 [Hanawalt et al., 1938]

References
Dorm, E. (1969). Acta Chem. Scand. 23, 1607.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.28	4	0 0 1	14.08
4.427	80	0 1 0	20.04
4.182	75	2 0 0	21.23
3.916	1	1 1 0	22.69
3.619	25	0 1 1	24.58
3.530	4	-2 0 1	25.21
3.432	25	2 0 1	25.94
3.342	7	-1 1 1	26.65
3.296	13	1 1 1	27.03
3.136	20	0 0 2	28.44
3.039	100	2 1 0	29.37
2.712	12	2 1 1	33.00
2.560	25	0 1 2	35.02
2.549	20	-2 0 2	35.18
2.473	7	2 0 2	36.29
2.468	7	-1 1 2	36.38
2.433	1L	1 1 2	36.92
2.359	2	3 1 0	38.12
2.228	2	-3 1 1	40.46
2.214	12	0 2 0	40.72
2.209	20	-2 1 2	40.82
2.189	2	3 1 1	41.21
2.159	6	2 1 2	41.81
2.139	1L	1 2 0	42.22
2.090M	20	4 0 0	43.25
2.090M		0 0 3	43.25
2.087	14	0 2 1	43.32
2.029	6	-1 2 1	44.63
2.021	5	1 2 1	44.81
2.002	1L	-4 0 1	45.27
1.964	4	4 0 1	46.18
1.956	7	2 2 0	46.38
1.8909M	16	0 1 3	48.08
1.8909M		4 1 0	48.08
1.8759	1	-2 2 1	48.49
1.8600	5	2 2 1	48.93
1.8561	4	-1 1 3	49.04
1.8487	6	2 0 3	49.25
1.8085	4	0 2 2	50.42
1.7958	6	4 1 1	50.80
1.7747	1	-1 2 2	51.45
1.7644	6	-4 0 2	51.77
1.7613	5	1 2 2	51.87
1.7413	5	-2 1 3	52.51
1.7333	1	3 2 0	52.77
1.7159	1	4 0 2	53.35
1.7055	6	2 1 3	53.70
1.6784	2	-3 2 1	54.64
1.6705	4	-2 2 2	54.92
1.6626	2	3 2 1	55.20

d(Å)	I	hkℓ			2θ(°)
1.6492	2	2	2	2	55.69
1.6386	6	-4	1	2	56.08
1.5992	1L	4	1	2	57.59
1.5684	1L	0	0	4	58.83
1.5643	1L	5	1	0	59.00
1.5286	1	-5	1	1	60.52
1.5188	4	4	2	0	60.95
1.5044	1	3	2	2	61.60
1.4893	1L	1	2	3	62.29
1.4838M	1L	-2	0	4	62.55
1.4838M		-4	2	1	62.55
1.4753	1L	0	3	0	62.95
1.4692	1	4	2	1	63.24
1.4561	1	4	0	3	63.88
1.4390	1	-2	2	3	64.73
1.4358	1	0	3	1	64.89
1.4222	1	-4	1	3	65.59
1.4174	3	-1	3	1	65.84
1.4138	2	1	3	1	66.03
1.4070	1	-2	1	4	66.39
1.3910	1	2	3	0	67.25
1.3831	2	4	1	3	67.69
1.3798	2	-4	2	2	67.87

Nicotinic Acid, $C_6H_5NO_2$

Synonym
1. 3-Pyridinecarboxylic Acid

CAS registry no.
59-67-6

Sample
The sample was NBS Standard Reference Material 148. It is used for checking microdeterminations of carbon, hydrogen and nitrogen.

Color
Colorless

Optical data
Biaxial(-), N_α = 1.424(2), N_β = 1.717, $N_\gamma \sim 1.79$.
2V = 46° [Wright and King, 1950].

Structure
Monoclinic, $P2_1/a$ (14), Z = 4, [Wright and King, 1950].

Lattice constants of this sample
a = 7.222(2) Å
b = 11.672(3)
c = 7.178(2)
β = 113.42(2)°

a/b = 0.6187
c/b = 0.6150

Volume
555.3 $Å^3$

Density
(calculated) 1.473 g/cm^3

Figure of merit
F_{30} = 47.8(0.011,57)

Reference intensity
$I/I_{corundum}$ = 0.95(3)

Additional pattern
1. PDF card 24-1843 [Wright and King, 1950]

Reference
Wright, W. B. and King, G. S. D. (1950). Acta Crystallogr. 3, 31.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ			2θ(°)
5.73	100	0	1	1	15.45
4.362	40	0	2	1	20.34
4.185	25	-1	2	1	21.21
3.743	7	1	1	1	23.75
3.588	55	-2	0	1	24.79
3.429	70	-2	1	1	25.96
3.314	80	2	0	0	26.88
3.271M	20	1	2	1	27.24
3.271M		-1	3	1	27.24
3.188	50	2	1	0	27.96
3.053	7	-2	2	1	29.23
3.043	8	-1	2	2	29.32
2.916M	3	0	4	0	30.63
2.916M		-2	1	2	30.63
2.881	3	2	2	0	31.01
2.869	3	0	2	2	31.15
2.773	4	1	3	1	32.26
2.670M	4	1	4	0	33.54
2.670M		0	4	1	33.54
2.628M	11	-1	3	2	34.09
2.628M		-1	4	1	34.09
2.513	6	0	3	2	35.70
2.381	5	-2	3	2	37.75
2.347	12	1	4	1	38.31
2.298	5	-2	0	3	39.16
2.259	7	-1	4	2	39.87
2.196	11	0	0	3	41.07
2.178	10	-1	5	1	41.43
2.157	3	0	1	3	41.85
2.145M	3	-3	2	2	42.09
2.145M		1	3	2	42.09
2.009	3	1	5	1	45.08
1.984	2	-3	3	2	45.68
1.977M	2	-3	1	3	45.86
1.977M		2	0	2	45.86
1.956	2	-2	5	1	46.37
1.949	1	2	1	2	46.56
1.928	1	1	4	2	47.09
1.905	1	0	5	2	47.71
1.866M	1	1	6	0	48.77
1.866M		0	6	1	48.77
1.8496M	1	-1	6	1	49.22
1.8496M		1	1	3	49.22
1.8094	3	-3	4	2	50.39
1.8064	4	-2	4	3	50.48
1.7833+	7	1	2	3	51.18
1.7833+		-2	0	4	51.18
1.7628+	3	-4	1	1	51.82
1.7628+		2	3	2	51.82

Oxalic Acid Hydrate, $C_2H_2O_4 \cdot 2H_2O$

Synonym
1. Ethanedioic acid dihydrate
2. Hydrogen oxalate hydrate

CAS registry no.
6153-56-6

Sample
Oxalic acid hydrate, analytical reagent was obtained from Mallinkrodt, St. Louis, MO 63147. It was dissolved in distilled water at room temperature. The solution was allowed to evaporate partly at room temperature and the precipitate was filtered.

Color
Colorless

Structure
Monoclinic, $P2_1/a$ (14), Z = 2. The structure was last refined by Ahmed and Cruickshank [1953] who correlated various earlier data.

Lattice constants of this sample
a = 11.890(3) Å
b = 3.6070(7)
c = 6.121(1)
β = 103.31(3)°

a/b = 3.2966
c/b = 1.6971

Volume
255.4 $Å^3$

Density
(calculated) 1.639 g/cm^3

Figure of merit
F_{30} = 52.8(0.012,47)

Additional pattern
1. PDF card 14-832 [de Wolff, Techn. Phys. Dienst, Delft, Holland]

Reference intensity
$I/I_{corundum}$ = 1.63(6)

Reference
Ahmed, F. R. and Cruickshank, D. W. J. (1953). Acta Crystallogr. 6, 385.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2Θ(°)
5.94	25	0 0 1	14.89
5.79	4	2 0 0	15.30
4.729	30	-2 0 1	18.75
3.737	1L	2 0 1	23.79
3.443	16	1 1 0	25.86
3.075	100	-1 1 1	29.01
2.937	10	-2 0 2	30.41
2.874	8	-4 0 1	31.09
2.632	1	3 1 0	34.03
2.595	4	2 1 1	34.53
2.562	4	-3 1 1	34.99
2.431	17	2 0 2	36.95
2.396	6	4 0 1	37.51
2.364	12	-4 0 2	38.03
2.333	2	-1 1 2	38.56
2.296	6	0 1 2	39.20
2.279M	12	3 1 1	39.51
2.279M		-2 1 2	39.51
2.257	8	4 1 0	39.92
2.178	1	1 1 2	41.42
1.986	3	0 0 3	45.65
1.978	3	-4 1 2	45.84
1.947	1L	5 1 0	46.61
1.929	2	6 0 0	47.08
1.8354	2	3 1 2	49.63
1.8210	1L	-6 0 2	50.05
1.8035	1L	0 2 0	50.57
1.7734	2	-1 1 3	51.49
1.7679	1	-2 1 3	51.66
1.7578	1L	2 0 3	51.98
1.7395	1	0 1 3	52.57
1.7236	2	-1 2 1	53.09
1.7218+	2	6 0 1	53.15
1.7218+		2 2 0	53.15
1.7011	1L	6 1 0	53.85
1.6915	1L	1 2 1	54.18
1.6710	2	1 1 3	54.90
1.6446	1	-4 1 3	55.86
1.6169	1	-3 2 1	56.90
1.5802	1	2 1 3	58.35
1.5422	2	0 2 2	59.93
1.5371M	3	3 2 1	60.15
1.5371M		-2 2 2	60.15
1.5307M	2	4 2 0	60.43
1.5307M		-2 0 4	60.43

Picric Acid, $C_6H_3N_3O_7$

Synonym
1. 2,4,6-Trinitrophenol

CAS registry no.
88-89-1

Sample
The sample was obtained from the General Chemical Division, Allied Chemical and Dye Corp., New York, NY. It was recrystallized from water.

Color
Light yellow

Structure
Orthorhombic, $P2_1ca$ (29), Z = 8 [Bredig and Möller, 1929].

Lattice constants of this sample
a = 9.723(4)Å
b = 19.139(6)
c = 9.271(3)

a/b = 0.5080
c/b = 0.4844

Volume
1725.3 Å^3

Density
(calculated) 1.764 g/cm^3

Figure of merit
F_{30} = 42.5(0.017,41)

Additional pattern
1. PDF card 9-789 [Morse and Baun, Wright Air Development Center, Wright-Patterson AFB, Ohio]

Reference
Bredig, M. A. and Möller, H. (1929). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 71, 331.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
9.56	20	0 2 0	9.24
6.65	3	0 2 1	13.31
6.38	6	0 3 0	13.88
6.34	6	1 1 1	13.96
5.49	45	1 2 1	16.13
5.245	1	0 3 1	16.89
4.784	40	0 4 0	18.53
4.706	15	2 1 0	18.84
4.629M	25	0 0 2	19.16
4.629M		1 3 1	19.16
4.507	11	0 1 2	19.68
4.327	16	2 2 0	20.51
4.247	19	0 4 1	20.90
4.184	20	1 0 2	21.22
4.087	19	1 1 2	21.73
3.901	90	1 4 1	22.78
3.869	100	2 3 0	22.97
3.831M	60	1 2 2	23.20
3.831M		0 5 0	23.20
3.750	70	0 3 2	23.71
3.569	30	2 3 1	24.93
3.500	45	1 3 2	25.43
3.411	19	2 4 0	26.10
3.351	14	2 0 2	26.58
3.326M	12	0 4 2	26.78
3.326M		1 5 1	26.78
3.203	4	2 4 1	27.83
3.191	5	0 6 0	27.94
3.152	13	1 4 2	28.29
3.015	90	0 6 1	29.61
2.954	7	0 5 2	30.23
2.944	9	0 2 3	30.34
2.909	7	1 1 3	30.71
2.879	25	1 6 1	31.04
2.862	40	2 5 1	31.23
2.822	9	1 5 2	31.68
2.815	13	1 2 3	31.76
2.780	6	0 3 3	32.17
2.673	25	1 3 3	33.50
2.667	27	2 6 0	33.57
2.626	8	0 6 2	34.11
2.597	9	0 4 3	34.51
2.576	11	3 4 1	34.80
2.564	11	2 6 1	34.96
2.532	6	1 7 1	35.42
2.523	5	2 5 2	35.56
2.509	9	1 4 3	35.76
2.411	3	4 1 0	37.27
2.389	3	3 5 1	37.62
2.355M	5	4 2 0	38.18

d(Å)	I	hkℓ	2θ(°)
2.355M		0 7 2	38.18
2.313	8	2 6 2	38.90
2.290M	2	2 4 3	39.32
2.290M		1 7 2	39.32
2.273	2	4 3 0	39.62
2.255M	3	1 0 4	39.94
2.255M		1 8 1	39.94
2.208M	3	3 6 1	40.83
2.208M		4 3 1	40.83
2.180M	2	0 3 4	41.39
2.180M		3 2 3	41.39
2.153	3	4 0 2	41.93
2.126M	9	0 8 2	42.49
2.126M		1 3 4	42.49
2.094	3	2 0 4	43.17
2.085	4	0 4 4	43.36
2.076	5	1 8 2	43.56
2.041+	5	3 6 2	44.35
2.041+		4 3 2	44.35
2.021	4	2 6 3	44.82
2.004M	3	1 7 3	45.22
2.004M		4 5 1	45.22
1.948M	4	2 9 0	46.58
1.948M		2 8 2	46.58
1.931	3	3 5 3	47.02

Potassium Chromium Sulfate, $KCr(SO_4)_2$

CAS registry no.
10141-00-1

Sample
The sample was prepared by heating $KCr(SO_4)_2 \cdot 12H_2O$ at 300 °C for several days. The crystallinity was improved by heating at 700 °C. However some impurity lines developed at this temperature, and therefore there may be minor errors in the intensities.

Color
Medium yellow green

Structure
Hexagonal, P321 (150), Z = 1, isostructural with other dehydrated alums such as $KAl(SO_4)_2$ and $NH_4Al(SO_4)_2$. The structure of these compounds was studied by Vegard and Maurstad [1928].

Lattice constants of this sample
a = 4.7547(6)Å
c = 8.054(2)

c/a = 1.6939

Volume
157.68 $Å^3$

Density
(calculated) 2.983 g/cm^3

Figure of merit
F_{19} = 74.6(0.010,25)

Additional pattern
1. PDF card 3-325 [Dow Chemical Co.]

Reference
Vegard L. and Maurstad, A. (1928). Z. Kristallogr, Kristallgeometrie Kristallphys. Kristallchem. 69, 519.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
8.06	40	0 0 1	10.97
4.115	15	1 0 0	21.58
3.664	100	1 0 1	24.27
2.879	75	1 0 2	31.04
2.685	10	0 0 3	33.34
2.377	35	1 1 0	37.81
2.280	8	1 1 1	39.50
2.0466	10	1 1 2	44.22
1.9948	4	2 0 1	45.43
1.8333	19	2 0 2	49.69
1.8085	13	1 0 4	50.42
1.7795	1	1 1 3	51.30
1.6110	2	0 0 5	57.13
1.5566	3	2 1 0	59.32
1.5364	10	1 1 4	60.18
1.5288	8	2 1 1	60.51
1.4514	13	2 1 2	64.11
1.4398	4	2 0 4	64.69
1.3724	12	3 0 0	68.29

Potassium Iron Sulfate (Yavapaiite), $KFe(SO_4)_2$

CAS registry no.
13718-65-5

Sample
The sample was precipitated by adding ethyl alcohol to a concentrated solution of KOH and $Fe(OH)_3$ in H_2SO_4.

Color
Colorless

Structure
Monoclinic, C2/m (12), Z = 2, [Hutton, 1959].

Lattice constants of this sample
a = 8.155(1)Å
b = 5.1539(6)
c = 7.877(1)
β = 94.85(1)°

a/b = 1.5823
c/b = 1.5284

Volume
329.9 Å^3

Density
(calculated) 2.890 g/cm^3

Figure of merit
F_{30} = 56.2(0.017,32)

Reference intensity
$I/I_{corundum}$ = 0.99(3)

Additional patterns
1. PDF card 12-632 [Hutton, 1959]
2. Corey and Sidhu [1945]

References
Hutton, C. O. (1959). Amer. Mineral. 44, 1105.
Corey, R. C. and Sidhu, S. S. (1945). J. Am. Chem. Soc. 67, 1490.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
7.87	70	0 0 1	11.23
4.354	11	1 1 0	20.38
4.066	50	2 0 0	21.84
3.885	70	-1 1 1	22.87
3.739M	65	-2 0 1	23.78
3.739M		1 1 1	23.78
3.494	55	2 0 1	25.47
2.985	100	-1 1 2	29.91
2.854	50	1 1 2	31.32
2.711	6	2 0 2	33.02
2.617	6	0 0 3	34.24
2.578	30	0 2 0	34.77
2.449	1	0 2 1	36.67
2.399	55	3 1 0	37.46
2.343	2	-3 1 1	38.39
2.288M	10	-2 0 3	39.34
2.288M		-1 1 3	39.34
2.197	3	1 1 3	41.04
2.176	1	2 2 0	41.46
2.154	13	0 2 2	41.91
2.120M	18	-2 2 1	42.61
2.120M		2 0 3	42.61
2.073	2	2 2 1	43.63
2.031	7	4 0 0	44.57
2.007	1	-4 0 1	45.13
1.980	2	3 1 2	45.79
1.963	3	0 0 4	46.22
1.941	13	-2 2 2	46.77
1.927	3	4 0 1	47.13
1.869M	12	-4 0 2	48.69
1.869M		2 2 2	48.69
1.837M	10	-3 1 3	49.58
1.837M		0 2 3	49.58
1.829	14	-2 0 4	49.81
1.821	6	-1 1 4	50.05
1.7597	6	1 1 4	51.92
1.7450	11	4 0 2	52.39
1.7111M	4	-2 2 3	53.51
1.7111M		2 0 4	53.51
1.7055	3	3 1 3	53.70
1.6801	2	1 3 0	54.58
1.6492	5	-1 3 1	55.69
1.5836	2	-4 2 1	58.21
1.5691	4	0 0 5	58.80
1.5609	4	0 2 4	59.14
1.5552	8	-1 3 2	59.38
1.5500	8	5 1 0	59.60
1.5353	4	1 3 2	60.23
1.5137	12	-4 2 2	61.18
1.4974M	5	5 1 1	61.92

Potassium Iron Sulfate (Yavapaiite), $KFe(SO_4)_2$ - (continued)

d(Å)	I	hkℓ			2θ(°)
1.4913	9	-2	2	4	62.20
1.4827	2	-5	1	2	62.60
1.4657	6	3	1	4	63.41
1.4510	9	3	3	0	64.13
1.4453	10	4	2	2	64.41
1.4251+	2	2	2	4	65.44
1.4251+		-1	3	3	65.44
1.4036M	5	-4	2	3	66.57
1.4036M		5	1	2	66.57
1.3538M	2	6	0	0	69.36
1.3538M		-6	0	1	69.36
1.3234	3	4	2	3	71.19
1.3078	2	0	0	6	72.17
1.2936	1	-3	3	3	73.09
1.2885M	6	5	1	3	73.43
1.2885M		0	4	0	73.43
1.2682	6	-1	1	6	74.80
1.2669	9	-5	1	4	74.89
1.2281	1	2	4	0	77.69
1.2184	1	-2	4	1	78.43
1.2157	4	2	0	6	78.64
1.2086	2	2	4	1	79.19
1.1990M	2	6	2	0	79.95
1.1990M		-6	2	1	79.95

Potassium Nitrosyl Ruthenium Chloride, $K_2NORuCl_5$

Sample
These data are essentially the same pattern reported by Swanson et al. [1963], with minor revisions. The pattern has been indexed using crystallographic data published since 1963. The very small sample used then was a special preparation and is no longer available. The original sample had been prepared from a mixture of a soluble ruthenium salt with KCl and concentrated HNO_3.

Color
Very dark red

Optical data
Biaxial(+), $N_\alpha = 1.750$, $N_\beta = 1.762$, $N_\gamma = 1.777$, $2V \sim 90°$

Structure
Orthorhombic, Pmnb (62), Z = 4 [Khodeshova and Bokii, 1964; de Wolff, 1968].

Lattice constants of this sample
a = 10.369(4)Å
b = 13.296(4)
c = 6.894(3)

a/b = 0.7798
c/b = 0.5185

Volume
950.4 Å^3

Density
(calculated) 2.701 g/cm^3

Figure of merit
$F_{30} = 54.6(0.018,31)$

Additional patterns
1. PDF card 24-886, revised by PDF editors [Swanson et al., 1963]
2. Powder Diffraction Data, [1976]. The data is very nearly the same as that given here.

References
Khodeshova, T. S. and Bokii, G. B. (1964). J. Struct. Chem. 5, 130.
Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976). (The Joint Committee on Powder Diffraction Standards, Swarthmore, PA, 19081), p. 387.
Swanson, H. E., Morris, M. C., Stinchfield, R. P., and Evans, E. H. (1963). Nat. Bur. Stand. U.S. Monogr. 25, Sec. 2, 29.
de Wolff, P. M. (1968). J. Appl. Crystallogr. 1, 108.

CuKα_1 λ = 1.540598 Å; temp 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.13	8	0 1 1	14.44
5.75	100	1 0 1	15.40
5.61	95	1 2 0	15.79
5.28	17	1 1 1	16.78
5.19	25	2 0 0	17.06
4.790	30	0 2 1	18.51
4.352	1L	1 2 1	20.39
4.085	6	2 2 0	21.74
3.962	10	2 1 1	22.42
3.731	4	0 3 1	23.83
3.520	25	2 2 1	25.28
3.509	25	1 3 1	25.36
3.450	25	0 0 2	25.80
3.335	16	0 1 2	26.71
3.325	16	0 4 0	26.79
3.176	1L	1 1 2	28.07
3.091	12	3 0 1	28.86
3.068	11	3 2 0	29.08
3.028	15	2 3 1	29.48
2.996	14	0 4 1	29.80
2.934	7	1 2 2	30.44
2.879	13	1 4 1	31.04
2.871	13	2 0 2	31.13
2.805	35	2 1 2	31.88
2.800M	35	3 2 1	31.94
2.800M		2 4 0	31.94
2.720	35	0 3 2	32.90
2.632M	8	2 2 2	34.03
2.632M		1 3 2	34.03
2.594M	50	2 4 1	34.55
2.594M		4 0 0	34.55
2.481	1L	0 5 1	36.18
2.409	7	2 3 2	37.29
2.393	10	0 4 2	37.56
2.277	15	4 2 1	39.54
2.262	10	3 4 1	39.82
2.238	4	2 5 1	40.26
2.211	10	1 1 3	40.78
2.167	1L	1 6 0	41.65
2.137	1L	3 3 2	42.26
2.105	7	0 5 2	42.93
2.072	14	4 0 2	43.66
2.063	16	1 5 2	43.84
2.047	6	4 1 2	44.22
2.037	7	2 6 0	44.44
2.000	4	1 3 3	45.30
1.980	10	5 2 0	45.78
1.959	4	4 4 1	46.32
1.954	4	2 6 1	46.44

Silver Thiocyanate, AgCNS

CAS registry no.
506-64-9

Sample
The sample was precipitated by adding $AgNO_3$ solution to one of KCNS.

Color
Colorless

Structure
Monoclinic, C2/c (15), Z = 8, [Lindqvist, 1957].

Lattice constants of this sample
a = 8.774(2) Å
b = 7.972(1)
c = 8.182(2)
β = 93.78(2)°

a/b = 1.1006
c/b = 1.0263

Volume
571.1 $Å^3$

Density
(calculated) 3.860 g/cm^3

Figure of merit
F_{30} = 54.6(0.014,39)

Reference intensity
$I/I_{corundum}$ = 2.95(9)

Additional pattern
1. PDF card 12-382 [Pistorius, University of California, Los Angeles, Calif.]

Reference
Lindqvist, J. (1957). Acta Crystallogr. 10, 29.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, A = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
5.890	65	1 1 0	15.03
4.674	100	1 1 1	18.97
4.079	5	0 0 2	21.77
3.577	25	0 2 1	24.87
3.426	3	-1 1 2	25.99
3.089	55	-2 0 2	28.88
2.945	10	2 2 0	30.33
2.891	12	2 0 2	30.91
2.850	9	0 2 2	31.36
2.810	19	-2 2 1	31.82
2.732	80	2 2 1	32.75
2.648	10	-3 1 1	33.82
2.542	14	1 3 0	35.28
2.512	13	-1 1 3	35.71
2.430	4	1 1 3	36.97
2.415	4	1 3 1	37.20
2.341	17	2 2 2	38.42
2.247	25	0 2 3	40.09
2.214	13	3 1 2	40.72
2.188	6	4 0 0	41.22
2.177	13	-1 3 2	41.44
2.140	4	1 3 2	42.20
2.046	4	-2 2 3	44.23
2.041	13	0 0 4	44.35
1.993M	2	-3 1 3	45.47
1.993M		0 4 0	45.47
1.965	2	3 3 0	46.15
1.9361	4	0 4 1	46.89
1.9191	4	4 2 0	47.33
1.9036	11	1 1 4	47.74
1.8991	11	-2 0 4	47.86
1.8920M	12	-4 2 1	48.05
1.8920M		3 3 1	48.05
1.8777	12	4 0 2	48.44
1.8737	8	3 1 3	48.55
1.8145	3	2 4 0	50.24
1.8051	5	2 0 4	50.52
1.7916	4	0 4 2	50.93
1.7818	4	-2 4 1	51.23
1.7607	2	2 4 1	51.89
1.7401	6	3 3 2	52.55
1.7105	1	5 1 0	53.53
1.6747	2	-2 4 2	54.77
1.6527	3	5 1 1	55.56
1.6405	5	2 4 2	56.01
1.6125	2	-4 2 3	57.07
1.6084	3	0 4 3	57.23
1.5772	2	1 3 4	58.47
1.5441M	2	-4 0 4	59.85
1.5441M		-1 5 1	59.85
1.5373	3	1 5 1	60.14
1.5275	4	4 2 3	60.57
1.4736	3	4 4 0	63.03
1.4618M	4	5 3 0	63.60
1.4618M		-4 4 1	63.60

Sodium Aluminum Fluoride (Chiolite), $Na_5Al_3F_{14}$

Sample
The sample was made by treating $NaHCO_3$ and Al powder with HF solution. The precipitate was dried and heated to 450 °C for 10 minutes.

Color
Colorless

Structure
Tetragonal, P4/mnc (128), Z = 2. The structure of $Na_5Al_3F_{14}$ was studied by Clausen [1936], and refined by Brosset [1938].

Lattice constants of this sample
a = 7.0142(8) Å
c = 10.400(3)

c/a = 1.4826

Volume
511.6 $Å^3$

Density
(calculated) 2.998 g/cm^3

Figure of merit
F_{30} = 61.2(0.014,35)

Reference intensity
$I/I_{corundum}$ = 1.15(5)

Additional pattern
1. PDF card 2-749 [Clausen, 1936] [Brosset, 1938]

References
Brosset, C., (1938). Z. Anorg. Allgem. Chem. 238, 201.
Clausen, H., (1936). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 95, 394.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
5.81	20	1 0 1	15.24
5.202	30	0 0 2	17.03
4.962	10	1 1 0	17.86
3.589	6	1 1 2	24.79
3.505	15	2 0 0	25.39
3.107	3	1 0 3	28.71
3.004	18	2 1 1	29.72
2.909	100	2 0 2	30.71
2.601	7	0 0 4	34.46
2.481	8	2 2 0	36.18
2.325	50	2 1 3	38.69
2.303	6	1 1 4	39.08
2.282	8	3 0 1	39.46
2.239	8	2 2 2	40.24
2.219	12	3 1 0	40.62
2.170	20	3 1 1	41.58
2.089	2	2 0 4	43.27
2.040	2	3 1 2	44.38
2.002	25	2 1 4	45.27
1.996	20	1 0 5	45.39
1.946	11	3 2 0	46.64
1.940	7	3 0 3	46.80
1.7939	25	2 2 4	50.86
1.7537	23	4 0 0	52.11
1.7340M	5	2 1 5	52.75
1.7340M		0 0 6	52.75
1.7020	2	4 1 0	53.82
1.6970	2	3 2 3	53.99
1.6875	6	3 1 4	54.32
1.6786	6	4 1 1	54.63
1.6615	3	4 0 2	55.24
1.6538	3	3 3 0	55.52
1.6167	6	4 1 2	56.91
1.5684	3	4 2 0	58.83
1.5538M	25	3 0 5	59.44
1.5538M		2 0 6	59.44
1.5013	19	4 2 2	61.74
1.4532M	7	4 0 4	64.02
1.4532M		1 0 7	64.02
1.4284	1	4 2 3	65.27
1.4208M	1	3 2 5	65.66
1.4208M		2 2 6	65.66
1.4023	2	4 3 0	66.64
1.3945	4	3 3 4	67.06

Sodium Borate, $Na_2B_4O_7$

CAS registry no.
1330-43-4

Sample
The sample was made by heating $Na_2B_4O_7 \cdot 10H_2O$ at 500 °C for 72 hours.

Color
Colorless

Structure
Triclinic, $P\bar{1}$ (2), Z = 4. The structure was refined by Krogh-Moe [1974].

Lattice constants of this sample
a = 8.646(4) Å
b = 10.506(4)
c = 6.572(2)
α = 94.95(2)°
β = 90.93(4)
γ = 93.18(3)
a/b = 0.8229
c/b = 0.6255

Volume
593.7 Å^3

Density
(calculated) 2.252 g/cm^3

Figure of merit
F_{30} = 44.4 (0.014,49)

Additional patterns
1. PDF card 9-14 [Dasgupta and Banerjee, 1955]
2. PDF card 27-656 [Smith et al., Annual Report to the Joint Committee on Powder Diffraction Standards, (1974)]

References
Dasgupta, D. R. and Banerjee, B. K. (1955). J. Chem. Phys. 23, 2189.
Krogh-Moe, J. (1974). Acta Crystallogr. B30, 578.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
10.46	7	0 1 0	8.45
8.64	5	1 0 0	10.23
6.55	20	0 0 1	13.51
6.49	35	1 1 0	13.63
5.78	10	0 -1 1	15.32
5.35	25	0 1 1	16.57
5.23	50	0 2 0	16.93
5.17	17	1 0 1	17.13
4.83	4	1 -1 1	18.34
4.77	4	-1 -1 1	18.58
4.64	8	-1 1 1	19.12
4.360	30	1 2 0	20.35
4.321	20	2 0 0	20.54
4.072	25	-2 1 0	21.81
3.926	100	0 2 1	22.63
3.879	12	1 -2 1	22.91
3.779	2	-1 -2 1	23.52
3.647	6	-1 2 1	24.39
3.484M	19	0 3 0	25.55
3.484M		2 -1 1	25.55
3.431+	35	-2 -1 1	25.95
3.431+		-2 1 1	25.95
3.297	30	-1 3 0	27.02
3.235	16	2 2 0	27.55
3.205	10	0 -1 2	27.81
3.086M	16	2 -2 1	28.91
3.086M		-1 0 2	28.91
3.035M	10	1 -3 1	29.41
3.035M		1 0 2	29.41
2.998	8	1 -1 2	29.78
2.972	8	0 3 1	30.04
2.859	11	-1 3 1	31.26
2.841	17	1 1 2	31.46
2.815	35	-3 1 0	31.76
2.790	20	-2 3 0	32.05
2.753	16	1 -2 2	32.50
2.670	45	0 2 2	33.54
2.580M	16	2 0 2	34.74
2.580M		-3 2 0	34.74
2.541	9	-1 4 0	35.29
2.513	15	-2 3 1	35.70
2.459M	50	1 4 0	36.51
2.459M		3 2 0	36.51
2.412	8	1 -3 2	37.25
2.374	6	-1 -4 1	37.87
2.287	8	0 3 2	39.37
2.240M	6	-1 3 2	40.22
2.240M		1 4 1	40.22
2.176	13	0 -1 3	41.47
2.160M	11	3 3 0	41.79
2.160M		4 0 0	41.79
2.134	16	0 -4 2	42.32
2.121M	20	-2 -4 1	42.60
2.121M		-2 4 1	42.60
2.087M	6	4 1 0	43.31
2.087M		1 -4 2	43.31
2.052	30	3 -2 2	44.10
2.040M	16	0 -5 1	44.37
2.040M		4 0 1	44.37
2.034M	16	-4 1 1	44.50
2.034M		-4 2 0	44.50
2.022	25	1 -2 3	44.79
1.936+	30	-4 2 1	46.90
1.936+		-1 4 2	46.90
1.923	25	-1 2 3	47.24

Sodium Borate, $Na_2B_4O_7$ (continued)

d(Å)	I	hkℓ	2θ(°)
1.882+	10	-4 3 0	48.33
1.882+		3 4 0	48.33
1.877	12	-3 4 1	48.45
1.870M	10	1 5 1	48.66
1.870M		-2 -2 3	48.66
1.865	10	2 1 3	48.80
1.837M	4	-3 3 2	49.59
1.837M		0 -5 2	49.59
1.821M	8	-4 0 2	50.05
1.821M		-2 4 2	50.05
1.807	13	-2 2 3	50.46
1.784	4	4 0 2	51.15
1.746	7	3 3 2	52.36
1.724	6	1 -4 3	53.09

Sodium Borate Hydroxide Hydrate (Borax), $Na_2B_4O_5(OH)_2 \cdot 8H_2O$

Synonym
1. Tincal

CAS registry no.
1303-96-4

Sample
The sample from Fisher Scientific Co., Fairlawn, NJ was recrystallized from aqueous solution. It was somewhat unstable in dry air, losing H_2O to become the 5-hydrate. Because of this instability it was impossible to obtain consistent results with the intensity measurements.

Color
Colorless

Structure
Monoclinic, A2/a (15), Z = 4. The structure of borax was studied by Morimoto [1956], and refined by Levy and Lisensky [1978] using neutron diffraction.

Lattice constants of this sample
a = 12.219(3) Å
b = 10.665(3)
c = 11.884(2)
β = 106.64(2)°

a/b = 1.1457
c/b = 1.1143

Volume
1483.8 Å^3

Density
(calculated) 1.709 g/cm^3

Figure of merit
F_{30} = 44.2(0.014,48)

Additional patterns
1. PDF card 12-258 [Cipriani, 1958]
2. PDF card 24-1055 [Thomas and Soustelle, 1970]
3. Minder, W. [1935]

References
Cipriani, C. (1958). Atti Soc. Toscana Sci. Natur. Pisa Mem. Processi Verb. Ser. A 65, 284.
Levy, H. A. and Lisensky, G. C. (1978). Acta Crystallogr. B34, 3502.
Minder, W. (1935). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 92, 301.
Morimoto, N. (1956). Mineral J. Japan 2, 1.
Thomas, G. and Soustelle, M. (1970). Bull. Soc. Chim. Fr. 1970, 4202.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
7.78	6	0 1 1	11.36
7.17	11	-1 1 1	12.34
5.97	16	1 1 1	14.83
5.84	40	2 0 0	15.15
5.69	50	0 0 2	15.56
5.33	7	0 2 0	16.61
5.20	20	-2 1 1	17.04
4.860	80	1 2 0	18.24
3.936M	45	-1 2 2	22.57
3.936M		2 2 0	22.57
3.889	1	0 2 2	22.85
3.596	7	2 0 2	24.74
3.577M	8	0 1 3	24.87
3.577M		-2 2 2	24.87
3.498M	5	-2 1 3	25.44
3.498M		1 2 2	25.44
3.391	2	0 3 1	26.26
3.334	3	-1 3 1	26.72
3.187M	8	1 3 1	27.97
3.187M		1 1 3	27.97
3.075	8	-3 2 2	29.01
2.980	40	2 2 2	29.96
2.929	10	4 0 0	30.50
2.848	65	0 0 4	31.39
2.833	60	2 3 1	31.55
2.740	1	2 1 3	32.66
2.676	4	-3 3 1	33.46
2.665	9	0 4 0	33.60
2.644M	5	-1 3 3	33.88
2.644M		-4 1 3	33.88
2.576	100	4 1 1	34.80
2.565M	95	-2 3 3	34.95
2.565M		4 2 0	34.95
2.520	2	3 2 2	35.60
2.459	11	3 3 1	36.51
2.387	4	-3 3 3	37.66
2.345	30	4 0 2	38.36
2.341	25	3 1 3	38.43
2.335	15	-2 4 2	38.53
2.313	5	2 0 4	38.91
2.258	1	-5 1 3	39.90
2.218	9	2 3 3	40.65
2.201M	8	3 4 0	40.97
2.201M		-4 2 4	40.97
2.174	5	-3 4 2	41.51
2.162	6	-4 3 3	41.74
2.146	8	4 2 2	42.07
2.122	2	2 2 4	42.56
2.098	4	0 5 1	43.09
2.081	10	-1 5 1	43.46

d(Å)	I	hkℓ	2θ(°)
2.076	7	-4 1 5	43.57
2.044	7	1 5 1	44.27
2.033	16	-6 0 2	44.52
2.015	8	4 1 3	44.96
1.989	2	3 3 3	45.58
1.983M	3	-1 4 4	45.71
1.983M		-4 4 2	45.71
1.969M	5	-1 3 5	46.05
1.969M		-2 3 5	46.05
1.950M	9	3 4 2	46.53
1.950M		6 0 0	46.53
1.913M	12	-3 3 5	47.50
1.913M		2 1 5	47.50
1.898	11	0 0 6	47.89
1.855M	9	5 3 1	49.08
1.855M		-2 2 6	49.08
1.833	12	6 2 0	49.71
1.790	4	-4 4 4	50.98
1.777M	5	4 3 3	51.39
1.777M		0 6 0	51.39
1.758M	10	-6 3 1	51.98
1.758M		1 6 0	51.98
1.748M	3	2 4 4	52.30
1.748M		-4 5 1	52.30
1.731	2	-6 3 3	52.84
1.705M	8	2 5 3	53.73
1.705M		2 3 5	53.73
1.701M	11	-7 1 3	53.84
1.701M		2 6 0	53.84
1.6613	2	-3 1 7	55.25
1.6585+	2	-7 2 2	55.35
1.6585+		1 6 2	55.35
1.6159M	2	-4 1 7	56.94
1.6159M		-6 4 2	56.94
1.5952	1	7 2 0	57.75
1.5841M	1	-1 5 5	58.19
1.5841M		-2 5 5	58.19
1.5740M	2	6 4 0	58.60
1.5740M		7 1 1	58.60
1.5457+	2	0 4 6	59.78
1.5457+		-5 1 7	59.78
1.5313M	2	-2 3 7	60.40
1.5313M		5 2 4	60.40
1.5197M	3	4 6 0	60.91
1.5197M		-3 3 7	60.91

d(Å)	I	hkℓ	2θ(°)
1.5177M	3	-1 3 7	61.00
1.5177M		-2 6 4	61.00
1.5083	3	0 6 4	61.42
1.4853	2	-4 3 7	62.48
1.4538	1	-4 0 8	63.99
1.4303M	5	6 3 3	65.17
1.4303M		-5 3 7	65.17
1.4233	4	0 0 8	65.53
1.4153	3	2 4 6	65.95
1.3608M	2	-5 2 8	68.95
1.3608M		-6 3 7	68.95

Sodium Silicon Fluoride (Malladrite), Na_2SiF_6

Sample
The sample was from Fisher Scientific Co., Fairlawn, NJ.

Color
Colorless

Structure
Hexagonal, P321 (150), Z = 3, isostructural with Na_2GeF_6 and other hexafluorides. The structure is similar to that of $K_2S_2O_6$. The structure of Na_2SiF_6 was determined by Zalkin et al. [1964].

Lattice constants of this sample
a = 8.8659(7) Å
c = 5.0433(5)

c/a = 0.5688

Volume
343.3 $Å^3$

Density
(calculated) 2.729 g/cm^3

Figure of merit
F_{30} = 76.6(0.012,34)

Reference intensity
$I/I_{corundum}$ = 0.87(2)

Additional patterns
1. PDF card 8-36 [African Explosives and Chem. Ind., Transvaal, South Africa]
2. PDF card 19-1193 [U.S. Bureau of Mines, Albany, OR]
3. PDF card 25-1166 [Royal Ontario Museum, Ontario, Canada], pattern is actually sylvite (KCl)
4. Cox [1954]
5. Cipriani [1955]

References
Cipriani, C. (1955). Rend. Soc. Mineral. Ital. 10, 253.
Cox, B. (1954). J. Chem. Soc. 1954, 3251.
Zalkin, A., Forrester, J. D., and Templeton, D. H. (1964). Acta Crystallogr. 17, 1408.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
5.041	13	0 0 1	17.58
4.429	100	1 1 0	20.03
4.213	95	1 0 1	21.07
3.331	90	1 1 1	26.74
3.056	50	2 0 1	29.20
2.902	9	2 1 0	30.79
2.558	5	3 0 0	35.05
2.521	7	0 0 2	35.58
2.516	15	2 1 1	35.66
2.394	1	1 0 2	37.54
2.281	90	3 0 1	39.47
2.216	6	2 2 0	40.68
2.191	4	1 1 2	41.16
2.129	3	3 1 0	42.42
2.107	4	2 0 2	42.88
2.030	9	2 2 1	44.61
1.9626	6	3 1 1	46.22
1.9043	10	2 1 2	47.72
1.7962	55	3 0 2	50.79
1.7616	4	3 2 0	51.86
1.6806	2	0 0 3	54.56
1.6629	20	3 2 1	55.19
1.6419	4	1 0 3	55.96
1.6269	9	3 1 2	56.52
1.5904	20	4 1 1	57.94
1.5718	4	1 1 3	58.69
1.5404	3	2 0 3	60.01
1.5268	3	4 0 2	60.60
1.4776	11	3 3 0	62.84
1.4695	5	5 0 1	63.23
1.4548	8	2 1 3	63.94
1.4514	8	4 2 0	64.11
1.4049	3	3 0 3	66.50
1.3951M	8	4 1 2	67.03
1.3951M		4 2 1	67.03
1.3391	1	2 2 3	70.23
1.3302	3	5 1 1	70.77
1.3194	2	3 1 3	71.44
1.2751	1	3 3 2	74.33
1.2643	2	4 0 3	75.07
1.2609	2	0 0 4	75.31
1.2293	4	5 2 0	77.60
1.2160	3	3 2 3	78.61
1.2099	2	5 1 2	79.09
1.1869	1	4 1 3	80.93
1.1566	1	2 1 4	83.52
1.1411	2	6 0 2	84.92
1.1312	3	3 0 4	85.84

Sodium Titanium Oxide, $Na_2Ti_3O_7$

CAS registry no.
12034-36-5

Sample
The sample was prepared by dry heating Na_2CO_3 + TiO_2 (anatase) at 1250 °C. Since Na evaporated, NaOH plus moisture was added to make a paste. The sample was then heated for 45 minutes at 1000 °C and then reheated for 17 hours at 950 °C after correcting with TiO_2.

Color
Colorless

Structure
Monoclinic, $P2_1/m$ (11), Z = 2. The structure was determined by Andersson and Wadsley [1961].

Lattice constants of this sample
a = 9.1279(7) Å
b = 3.8032(5)
c = 8.5621(7)
β = 101.60(1)°

a/b = 2.4001
c/b = 2.2513

Volume
291.17 Å^3

Density
(calculated) 3.441 g/cm^3

Figure of merit
F_{30} = 115.3(0.008,32)

Additional pattern
1. PDF card 14-85 [Andersson and Wadsley, 1961]

Reference
Andersson, S. and Wadsley, A. D. (1961). Acta Crystallogr. 14, 1245.

CuKα_1 λ = 1.540598 Å; temp 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
8.95	7	1 0 0	9.87
8.40	100	0 0 1	10.52
6.84	4	-1 0 1	12.93
5.587	30	1 0 1	15.85
4.469	7	2 0 0	19.85
4.189	2	0 0 2	21.19
4.130	5	-1 0 2	21.50
3.652	2	2 0 1	24.35
3.535	1	1 0 2	25.17
3.464	35	0 1 1	25.70
3.422	5	-2 0 2	26.02
3.142	18	1 1 1	28.38
3.005	7	-3 0 1	29.71
2.982	20	3 0 0	29.94
2.897	6	2 1 0	30.84
2.856	7	-2 1 1	31.29
2.817	8	0 1 2	31.74
2.799M	12	-1 1 2	31.95
2.799M		0 0 3	31.95
2.791	7	2 0 2	32.04
2.699	5	-3 0 2	33.16
2.645	8	3 0 1	33.86
2.635	9	2 1 1	34.00
2.618	16	-2 0 3	34.22
2.588	7	1 1 2	34.63
2.543	6	-2 1 2	35.26
2.527	6	1 0 3	35.49
2.358	3	-3 1 1	38.13
2.346	4	3 1 0	38.33
2.282	1	-3 0 3	39.46
2.274	1L	-1 1 3	39.60
2.251M	1	0 1 3	40.02
2.251M		2 1 2	40.02
2.236	2	4 0 0	40.31
2.172	2	3 1 1	41.54
2.158	1	-2 1 3	41.82
2.1050	3	1 1 3	42.93
2.0967	4	0 0 4	43.11
2.0643	35	-2 0 4	43.82
2.0598	40	4 0 1	43.92
1.9558M	6	-3 1 3	46.39
1.9558M		1 0 4	46.39
1.9271	2	4 1 0	47.12
1.9221	1	3 1 2	47.25
1.9009	20	0 2 0	47.81
1.8607M	2	3 0 3	48.91
1.8607M		1 2 0	48.91
1.8547	3	0 2 1	49.08
1.8261M	2	4 0 2	49.90
1.8261M		-5 0 1	49.90

Sodium Titanium Oxide, $Na_2Ti_3O_7$ - (continued)

d(Å)	I	hkℓ			2θ(°)
1.8149	10	-2	1	4	50.23
1.8105	7	4	1	1	50.36
1.7998	2	1	2	1	50.68
1.7670	1	2	0	4	51.69
1.7333	1	-4	1	3	52.77
1.7279	1L	-1	2	2	52.95
1.7120	1	-1	0	5	53.48
1.6815	1	5	0	1	54.53
1.6716	1	3	1	3	54.88
1.6663	3	-5	0	3	55.07
1.6459+	7	4	1	2	55.81
1.6459+		-5	1	1	55.81
1.6112	2	-5	1	2	57.12
1.6071M	3	-3	2	1	57.28
1.6071M		-3	0	5	57.28
1.6030M	5	3	2	0	57.44
1.6030M		2	1	4	57.44
1.5964	2	4	0	3	57.70
1.5797	1	-1	2	3	58.37
1.5612	5	-1	1	5	59.13
1.5413	6	-2	1	5	59.97
1.5378M	6	5	1	1	60.12
1.5378M		5	0	2	60.12
1.5195M	4	-5	0	4	60.92
1.5195M		1	2	3	60.92
1.5024	2	-6	0	2	61.69
1.4934	1	-4	0	5	62.10
1.4902	1	6	0	0	62.25
1.4759	4	2	0	5	62.92
1.4720	6	4	1	3	63.11
1.4410	6	-6	0	3	64.63
1.4257M	2	-1	0	6	65.41
1.4257M		5	1	2	65.41
1.4117M	5	-6	1	1	66.14
1.4117M		-5	1	4	66.14
1.3980M	14	-2	2	4	66.87
1.3980M		0	0	6	66.87
1.3969M	14	-6	1	2	66.93
1.3969M		4	2	1	66.93
1.3874	1	6	1	0	67.45
1.3759M	6	-3	0	6	68.09
1.3759M		2	1	5	68.09
1.3631	2	1	2	4	68.82
1.3507	1	3	0	5	69.54
1.3473	1L	-6	1	3	69.74
1.3347	1	-1	1	6	70.50

Strontium Chromium Oxide, Sr_2CrO_4

CAS registry no.
12206-20-1

Sample
The sample was made by heating Cr_2O_3 with $SrCrO_4$ and $Sr(OH)_2$ under N_2 at about 1000 °C for about 1/2 hour.

Color
Black

Structure
Orthorhombic, $P2_1nb$ (33), Z = 8. The structure of Sr_2CrO_4 has been studied by Wilhelmi [1967].

Lattice constants of this sample
a = 10.007(2) Å
b = 14.194(3)
c = 5.809(1)

a/b = 0.7050
c/b = 0.4093

Volume
825.1 $Å^3$

Density
(calculated) 4.689 g/cm^3

Figure of merit
F_{30} = 66.2(0.012,38)

Polymorphism
Kafalas and Longo [1972] report that Sr_2CrO_4 transforms to a K_2NiF_4 structure at 65 kbars and 1000 °C.

Additional pattern
1. PDF card 19-1206 [Wilhelmi, 1967]

References
Kafalas, J. A. and Longo, J. M. (1972). J. Solid State Chem. 4, 55.
Wilhelmi, K.-A., (1967). Ark. Kemi 26, 157.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
5.024	3	1 0 1	17.64
5.007	2	2 0 0	17.70
3.663M	4	0 3 1	24.28
3.663M		2 1 1	24.28
3.448	3	1 3 1	25.82
3.343M	17	1 4 0	26.64
3.343M		2 2 1	26.64
3.029	19	0 4 1	29.47
3.021	16	3 2 0	29.54
2.901	90	1 4 1	30.80
2.892M	100	2 4 0	30.89
2.892M		3 0 1	30.89
2.848	8	0 1 2	31.39
2.738	2	1 1 2	32.68
2.680	1	3 2 1	33.41
2.592	5	2 4 1	34.58
2.550	2	0 5 1	35.16
2.512	3	2 0 2	35.72
2.472M	4	2 1 2	36.31
2.472M		1 5 1	36.31
2.430	20	3 4 0	36.96
2.403	2	1 3 2	37.39
2.368M	5	2 2 2	37.97
2.368M		0 6 0	37.97
2.360	6	4 2 0	38.10
2.303	7	1 6 0	39.09
2.273	1	2 5 1	39.61
2.267	1	4 1 1	39.72
2.247	1	0 4 2	40.10
2.243	1L	3 4 1	40.18
2.219	6	2 3 2	40.63
2.193M	5	1 4 2	41.13
2.193M		0 6 1	41.13
2.187	8	4 2 1	41.25
2.165	3	3 1 2	41.69
2.139	3	2 6 0	42.22
2.092	6	3 2 2	43.20
2.050	18	2 4 2	44.15
1.9878	3	3 3 2	45.60
1.9252	9	5 2 0	47.17
1.8916	4	5 0 1	48.06
1.8791	3	4 1 2	48.40
1.8636	9	3 4 2	48.83
1.8344	1	0 6 2	49.66
1.8038	2	1 6 2	50.56
1.7916M	3	0 3 3	50.93
1.7916M		2 1 3	50.93
1.7743	1	0 8 0	51.46
1.7641	3	1 3 3	51.78
1.7500	4	2 2 3	52.23

Strontium Chromium Oxide, Sr_2CrO_4 - (continued)

d(Å)	I	hkℓ	2θ(°)
1.7438	5	5 4 0	52.43
1.7340	3	3 5 2	52.75
1.7221	1	2 6 2	53.14
1.6996	3	0 4 3	53.90
1.6872	1	2 3 3	54.33
1.6744	11	3 0 3	54.78
1.6716	13	4 4 2	54.88
1.6632M	6	3 1 3	55.18
1.6632M		0 7 2	55.18
1.6486	7	4 6 1	55.71
1.6368	2	5 1 2	56.15
1.6087	7	2 4 3	57.22
1.6058	4	5 2 2	57.33
1.5789M	2	1 5 3	58.40
1.5789M		3 3 3	58.40
1.5658	5	3 8 0	58.94
1.5636	2	6 2 1	59.03

Thallium, α-Tl

CAS registry no.
7440-28-0

Sample
The sample was obtained from the Fisher Scientific Co., Silver Spring, MD.

Color
Gray metallic

Structure
Hexagonal, $P6_3/mmc$ (194), Z = 2, isostructural with magnesium. The structure of thallium was studied by Sekito [1930].

Lattice constants of this sample
a = 3.4568(3) Å
c = 5.5259(5)

c/a = 1.5986

Volume
57.185 Å^3

Density
(calculated) 11.869 g/cm^3

Figure of merit
F_{22} = 76.9(0.012,24)

Polymorphism
Hexagonal thallium transposes to a body-centered cubic phase above 230 °C [Lipson and Stokes, 1941]. Becker and Ebert [1923] had reported a tetragonal phase which later was shown to be hexagonal.

Additional patterns
1. PDF 1-1084 [Hanawalt et al., 1938]
2. Barrett [1958]
3. Sekito [1930]
4. Suganuma [1960]

References

Barrett, C. S. (1958). Phys. Rev. 110, 1071.
Becker, K. and Ebert, F. (1923). Z. Phys. 16, 165.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Lipson, H. and Stokes, A. R. (1941). Nature 148, 437.
Sekito, S. (1930). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 74, 189.
Suganuma, R. (1960). J. Phys. Soc. Japan. 15, 1395.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C Internal standard W, a = 3.16524 Å					
d(Å)	I	h	k	ℓ	2θ(°)
2.991	20	1	0	0	29.85
2.760	50	0	0	2	32.41
2.631	100	1	0	1	34.05
2.030	20	1	0	2	44.59
1.7285	18	1	1	0	52.93
1.5687	35	1	0	3	58.82
1.4965	3	2	0	0	61.96
1.4651	20	1	1	2	63.44
1.4447	14	2	0	1	64.44
1.3820	8	0	0	4	67.75
1.3159	3	2	0	2	71.66
1.2544	7	1	0	4	75.77
1.1617	9	2	0	3	83.07
1.1084	10	2	1	1	88.05
1.0792	11	1	1	4	91.09
1.0473	2	2	1	2	94.70
1.0368	16	1	0	5	95.97
1.0151	3	2	0	4	98.72
.9980	3	3	0	0	101.04
.9640	6	2	1	3	106.08
.9386	3	3	0	2	110.30
.9210	3	0	0	6	113.52

Thallium Fluoride, TlF

CAS registry no.
7789-27-7

Sample
The sample was obtained from the City Chemical Co., New York, NY.

Color
Colorless

Structure
Orthorhombic, Z = 4. Pca* is consistent with the absences and has been used without any verifying data. Ketelaar [1935] determined that TlF belonged to the space group Fmmm (69). However, data reported here, as well as data from another researcher, Harshaw (priv. comm.), have a number of weak extra lines which do not fit that space group. These extra lines were found to persist after the sample had been refluxed.

Lattice constants of this sample
a = 5.4910(4) Å
b = 6.0974(3)
c = 5.1855 (4)

a/b = 0.9006
c/b = 0.8504

Volume
173.61 Å^3

Density
(calculated) 8.546 g/cm^3

Figures of merit
F_{30} = 44.6(0.010,70)
M_{20} = 71.0

Reference intensity
$I/I_{corundum}$ = 3.2(3)

Additional pattern
1. PDF 3-0483 [Ketelaar, 1935]

Reference
Ketelaar, J. A. A. (1935). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 92, 30.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
6.095	1	0 1 0	14.52
3.205	100	1 1 1	27.81
3.047	45	0 2 0	29.29
2.748	16	2 0 0	32.56
2.593	16	0 0 2	34.56
2.426	1	2 0 1	37.02
2.370	2	1 2 1	37.93
2.0400	13	2 2 0	44.37
1.9755	11	0 2 2	45.90
1.8857	11	2 0 2	48.22
1.7889	20	1 3 1	51.01
1.6604	8	3 1 1	55.28
1.6033	10	2 2 2	57.43
1.5916	8	1 1 3	57.89
1.5243	4	0 4 0	60.71
1.4134	1L	1 4 1	66.05
1.3727	1	4 0 0	68.27
1.3327	3	2 4 0	70.62
1.3143	5	0 4 2	71.76
1.2965M	1	4 1 1	72.90
1.2965M		0 0 4	72.90
1.2807	4	1 3 3	73.95
1.2517	1	4 2 0	75.96
1.2307	3	3 1 3	77.50
1.2194	1L	0 5 0	78.35
1.2129	1	4 0 2	78.85
1.1930	1	0 2 4	80.43
1.1897	1	4 1 2	80.70
1.1854	3	2 4 2	81.06
1.1717	1	3 4 0	82.21
1.1601	4	1 5 1	83.21
1.1273	1	4 2 2	86.21
1.1111	1L	4 3 1	87.78
1.1037	1L	0 5 2	88.52
1.0940	2	2 2 4	89.52
1.0690	2	3 3 3	92.20
1.0583	2	5 1 1	93.42
1.0201	1	4 4 0	98.07
1.0164	1	0 6 0	98.56
.9959	1	3 5 1	101.33
.9876	1L	0 4 4	102.52
.9805	1	1 5 3	103.55
.9719	1L	1 4 4	104.85
.9530	1	2 6 0	107.85
.9493	1	4 4 2	108.47
.9461	1	0 6 2	109.01
.9291	1	2 4 4	112.00
.9111	1	1 3 5	115.45
.9004	1	4 2 4	117.64
.8945	1	2 6 2	118.89
.8751	1	3 5 3	123.34
.8486	1	1 7 1	130.38

Thallium Hydrogen Phthalate, $C_8H_5O_4Tl$

Synonyms
1. Thallous acid phthalate
2. Thallium hydrogen-o-phthalate

CAS registry no.
29050-41-7

Sample
The sample was obtained as fragments of a single crystal, originally from Quartz Products, Plainfield, NJ.

Color
Colorless

Structure
Orthorhombic, $Pca2_1$ (29), Z = 4, by analogy with $C_8H_5O_4Rb$. The structure of $C_8H_5O_4Rb$ was refined by Smith [1975].

Lattice constants of this sample
a = 10.050(2) Å
b = 12.882(2)
c = 6.622(1)

a/b = 0.7802
c/b = 0.5140

Volume
857.2 Å^3

Density
(calculated) 2.863 g/cm^3

Figure of merit
F_{30} = 54.7(0.014,40)

Reference
Smith, R. A. (1975). Acta Crystallogr. B31, 2347.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
12.91	100	0 1 0	6.84
7.91	1L	1 1 0	11.18
6.44	11	0 2 0	13.73
5.43	3	1 2 0	16.32
5.084	4	1 1 1	17.43
5.029	2	2 0 0	17.62
4.684	1	2 1 0	18.93
4.296	3	0 3 0	20.66
4.197	4	1 2 1	21.15
4.005	12	2 0 1	22.18
3.952	9	1 3 0	22.48
3.824	25	2 1 1	23.24
3.397	25	2 2 1	26.21
3.311	2	0 0 2	26.91
3.220	10	0 4 0	27.68
3.066	5	1 4 0	29.10
2.972	4	3 2 0	30.04
2.944	8	0 2 2	30.34
2.930	7	2 3 1	30.48
2.825	3	1 2 2	31.65
2.783	6	1 4 1	32.14
2.708M	2	3 2 1	33.05
2.708M		2 4 0	33.05
2.643	3	3 3 0	33.89
2.624	2	0 3 2	34.14
2.577	1L	0 5 0	34.78
2.538	2	1 3 2	35.34
2.510M	4	4 0 0	35.74
2.510M		2 4 1	35.74
2.496	2	1 5 0	35.95
2.466	3	4 1 0	36.41
2.336	7	1 5 1	38.51
2.323M	4	2 3 2	38.73
2.323M		3 4 0	38.73
2.250	2	1 4 2	40.05
2.210	3	3 2 2	40.79
2.169	1L	4 3 0	41.61
2.147	1L	0 6 0	42.05
2.099	1L	1 6 0	43.05
2.063	3	3 3 2	43.84
2.060	2	4 3 1	43.91
2.042	3	3 5 0	44.32
2.021	2	2 0 3	44.80
2.001	6	1 6 1	45.28
1.997	6	2 1 3	45.38
1.978	3	4 1 2	45.85
1.952	1L	3 5 1	46.48
1.927M	2	2 2 3	47.12
1.927M		1 3 3	47.12
1.911	2	4 2 2	47.54

Thallium Hydrogen Phthalate, $C_8H_5O_4Tl$ - (continued)

d(Å)	I	hkℓ			2θ(°)
1.901M	3	5	1	1	47.80
1.901M		3	4	2	47.80
1.840	1L	0	7	0	49.49
1.829	1	2	3	3	49.82
1.809	2	1	7	0	50.40
1.792	1	1	4	3	50.93
1.773	1L	1	6	2	51.49
1.755	1	5	3	1	52.07
1.746	1	1	7	1	52.35
1.7392	2	3	5	2	52.58
1.6996	1L	4	4	2	53.90
1.6953	1L	2	6	2	54.05
1.6713	1L	2	7	1	54.89
1.6522M	2	1	5	3	55.58
1.6522M		5	4	1	55.58
1.6416	1	0	1	4	55.97
1.6198M	1L	6	2	0	56.79
1.6198M		1	1	4	56.79
1.6094M	1	0	8	0	57.19
1.6094M		0	7	2	57.19
1.5861	1	3	6	2	58.11
1.5455M	1	1	8	1	59.79
1.5455M		0	3	4	59.79
1.5415	1	5	5	1	59.96
1.5209	1L	1	6	3	60.86
1.4937	1L	2	8	1	62.09
1.4842M	1L	6	1	2	62.53
1.4842M		4	7	0	62.53

Thallium Oxide (Avicennite), Tl_2O_3

The experimental data reported here are the same as those reported earlier by Swanson and Fuyat [1953]. This pattern has not been re-measured. The space group has been changed and the corresponding indices were changed when necessary. Also other additional information has been added.

CAS registry no.
1314-12-1

Sample
The sample of thallium oxide from Johnson Matthey Co., Ltd., London, England, was annealed at 370 °C in a sealed tube for 2 hours to prevent volatilization of noxious fumes.

Major impurities
0.001 to 0.01% each: Ca, Mg, Li, and Na
less than 0.001% each: Al, Cu, Pb, and Si.

Color
Black

Structure
Cubic, Ia3 (206), Z = 16, isostructural with Mn_2O_3 [Pauling and Shappell, 1930]. The space group used earlier was $I2_13$.

Lattice constant of this sample
a = 10.5434(7) Å

Volume
1172.0 $Å^3$

Density
(calculated) 10.354 g/cm^3

Figure of merit
F_{30} = 52.7(0.018,31)

Polymorphism
Prewitt et al. [1969] report the existence of a hexagonal modification.

Additional patterns
1. PDF card 5-584 [Swanson and Fuyat, 1953]
2. Hanawalt et al. [1938]
3. Kon'kova and Savel'ev [1960], natural mineral

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Kon'kova, E. A. and Savel'ev, V. F. (1960). Zap. Vses. Mineral. Obshchest. 89, 316.
Pauling, L. and Shappell, M. D. (1930). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 75, 128.
Prewitt, C. T., Shannon, R. D., Rogers, D. B., and Sleight, A. W. (1969). Inorg. Chem. 8, 1985.
Swanson, H. E. and Fuyat, R. K. (1953). Nat. Bur. Stand. U.S. Circ. 539, 2, 28.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
4.304	11	2 1 1	20.62
3.042	100	2 2 2	29.34
2.816	3	3 2 1	31.75
2.635	42	4 0 0	34.00
2.484	6	4 1 1	36.13
2.357	2	4 2 0	38.15
2.248	4	3 3 2	40.08
2.149	1	4 2 2	42.01
2.068	8	4 3 1	43.74
1.924	3	5 2 1	47.20
1.863	33	4 4 0	48.85
1.808	2	4 3 3	50.43
1.758	1	6 0 0	51.97
1.710	5	6 1 1	53.55
1.668	2	6 2 0	55.01
1.6280	4	5 4 1	56.48
1.5890	27	6 2 2	57.99
1.5540	6	6 3 1	59.43
1.5220	6	4 4 4	60.81
1.4910	3	5 4 3	62.21
1.4620	1	6 4 0	63.59
1.4340	3	6 3 3	64.98
1.4090	2	6 4 2	66.28
1.3390	3	6 5 1	70.24
1.3180	3	8 0 0	71.53
1.2980	4	7 4 1	72.80
1.2790	2	8 2 0	74.06
1.2597	2	6 5 3	75.40
1.2428	1	6 6 0	76.60
1.2261	3	8 3 1	77.84
1.2094	6	6 6 2	79.13
1.1789	4	8 4 0	81.60
1.1646	1	8 3 3	82.82
1.1371	2	9 2 1	85.29
1.1110	1	7 5 4	87.79
1.0874	1	9 3 2	90.21
1.0764	2	8 4 4	91.39
1.0649	1	9 4 1	92.66

Uric Acid (Phase 1), $C_5H_4N_4O_3$

Synonyms
1. 2,6,8-Trioxypurine
2. 8-Hydroxyxanthine

CAS registry no.
69-93-2

Sample
The sample was NBS Standard Reference Material 913.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14), Z = 4. The structure was determined by Ringertz [1966].

Lattice constants of this sample
a = 13.102(3) Å
b = 7.416(2)
c = 6.225(1)
β = 90.37(3)°

a/b = 1.7667
c/b = 0.8394

Volume
604.9 Å^3

Density
(calculated) 1.846 g/cm^3

Figure of merit
F_{30} = 36.3(0.012,68)

Reference intensity
$I/I_{corundum}$ = 0.94(1)

Polymorphism
Shirley and Sutor [1968] report a second phase with a monoclinic cell of similar size.

Additional patterns
1. PDF card 21-1959 [Shirley and Sutor, 1968]
2. PDF card 22-2000 [Swanson et al., 1970]

References
Ringertz, H. (1966). Acta Crystallogr. 20, 397.
Shirley, R. and Sutor, D. J. (1968). Science 159, 544.
Swanson, H. E., McMurdie, H. F., Morris, M. C., and Evans, E. H. (1970). Nat. Bur. Std. U.S. Monogr. 25, Sec. 8, 154.

CuKα$_1$ λ = 1.540598 Å; temp 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.54	45	2 0 0	13.53
5.633	18	-1 0 1	15.72
4.913	50	2 1 0	18.04
4.769	7	0 1 1	18.59
4.485	2	-1 1 1	19.78
3.860	55	-2 1 1	23.02
3.706	7	0 2 0	23.99
3.587	4	-3 0 1	24.80
3.276	17	4 0 0	27.20
3.185	50	0 2 1	27.99
3.098	100	-1 2 1	28.79
2.994	4	4 1 0	29.82
2.868M	25	0 1 2	31.16
2.868M		-2 2 1	31.16
2.801	11	1 1 2	31.93
2.623	3	2 1 2	34.15
2.570	16	3 2 1	34.88
2.456	3	4 2 0	36.56
2.421	4	-5 0 1	37.11
2.312	4	2 3 0	38.92
2.280	5	4 2 1	39.50
2.245	11	-2 2 2	40.14
2.184	6	6 0 0	41.31
2.151M	2	4 1 2	41.96
2.151M		3 3 0	41.96
2.096M	2	-3 2 2	43.12
2.096M		6 1 0	43.12
2.032	3	3 3 1	44.56
2.027	3	-5 2 1	44.67
1.997	1L	0 1 3	45.37
1.989	1L	-6 1 1	45.56
1.978	1L	-1 1 3	45.84
1.9306M	1	-4 2 2	47.03
1.9306M		5 1 2	47.03
1.9149+	1	-2 1 3	47.44
1.9149+		1 3 2	47.44
1.8821M	2	-4 3 1	48.32
1.8821M		6 2 0	48.32
1.8788M	2	-3 0 3	48.41
1.8788M		4 3 1	48.41
1.8697	1	3 0 3	48.66
1.7988M	6	6 2 1	50.71
1.7988M		5 3 0	50.71
1.7955M	5	-7 0 1	50.81
1.7955M		-1 2 3	50.81

Zinc Chlorate Hydrate, $Zn(ClO_4)_2 \cdot 6H_2O$

CAS registry no.
13637-61-1

Sample
The sample was prepared by evaporation at room temperature of an aqueous solution.

Color
Colorless

Structure
Hexagonal, P6/mmm (191), Z = 4, isostructural with Ni and other divalent metal perchlorate hexahydrates. The structure of this group of compounds was studied by West [1935].

Lattice constants of this sample
a = 15.629(4) Å
c = 5.215(1)

c/a = 0.3337

Volume
1103.1 $Å^3$

Density
(calculated) 2.242 g/cm^3

Figure of merit
F_{30} = 32.3(0.012,77)

Additional pattern
1. PDF card 6-197 [Dow Chemical Co.]

Reference
West, C. D. (1935). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 91, 480.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
6.77	6	2 0 0	13.06
4.868	14	1 0 1	18.21
4.341	6	1 1 1	20.44
4.132	85	2 0 1	21.49
3.909	100	2 2 0	22.73
3.655	6	2 1 1	24.33
3.386	3	4 0 0	26.30
3.045	2	3 1 1	29.31
2.841	75	4 0 1	31.46
2.670	3	3 2 1	33.54
2.608	12	0 0 2	34.36
2.560M	3	1 0 2	35.03
2.560M		4 2 0	35.03
2.433M	10	2 0 2	36.91
2.433M		5 1 0	36.91
2.296	11	4 2 1	39.21
2.258M	6	3 0 2	39.90
2.258M		6 0 0	39.90
2.168M	4	2 2 2	41.62
2.168M		5 2 0	41.62
2.072	8	6 0 1	43.66
2.066M	18	4 0 2	43.79
2.066M		6 1 0	43.79
1.955M	12	4 1 2	46.42
1.955M		4 4 0	46.42
1.878M	6	5 0 2	48.42
1.878M		6 2 0	48.42
1.826	22	4 2 2	49.91
1.7657	9	6 2 1	51.73
1.7058M	5	6 0 2	53.69
1.7058M		6 3 0	53.69
1.6950	2	7 1 1	54.06
1.6838	4	2 0 3	54.45
1.6089	2	8 0 1	57.21
1.5462	5	4 0 3	59.76
1.5236M	4	6 2 2	60.74
1.5236M		7 3 0	60.74
1.4768M	7	7 1 2	62.88
1.4768M		8 2 0	62.88
1.4626	1L	5 0 3	63.56
1.4372	1	4 2 3	64.82
1.4193M	4	8 0 2	65.74
1.4193M		6 5 0	65.74

Zinc Phosphate, α -$Zn_3(PO_4)_2$

CAS registry no.
7779-90-0

Sample
The sample was prepared by heating $ZnCO_3$ and P_2O_5 at 900 °C for several days with intermittent grindings.

Color
Colorless

Structure
Monoclinic, A2/a (15), Z = 4. The structure was determined by Calvo [1965].

Lattice constants of this sample
a = 15.006(3) Å
b = 5.635(1)
c = 8.183(1)
β = 104.99(2)°

a/b = 2.6629
c/b = 1.4521

Volume
668.5 $Å^3$

Density
3.836 g/cm^3

Figure of merit
F_{30} = 37.4(0.016,51)

Reference intensity
$I/I_{corundum}$ = 1.40(9)

Polymorphism
Above 942 °C, α - $Zn_3(PO_4)_2$ transforms to β - $Zn_3(PO_4)_2$. A small percentage of Mn++ substituting for the Zn++ stabilizes a γ form [Calvo, 1965].

Additional patterns
1. PDF card 1-524 [New Jersey Zinc Co.]
2. PDF card 11-35 [Katnack and Hummel, 1958]

References
Calvo, C. (1965). Can. J. Chem. 43, 436.
Katnack, F. L. and Hummel, F. A. (1958). J. Electrochem. Soc. 105, 125.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I	hkℓ	2θ(°)
7.25	3	2 0 0	12.20
4.583M	35	0 1 1	19.35
4.583M		-1 1 1	19.35
4.193	30	1 1 1	21.17
3.947	35	0 0 2	22.51
3.928	25	-2 0 2	22.62
3.607	90	-3 1 1	24.66
3.146	70	2 0 2	28.35
3.079	100	-4 1 1	28.98
2.815	13	0 2 0	31.76
2.764	9	1 2 0	32.36
2.657	9	4 1 1	33.70
2.627	20	2 2 0	34.10
2.448	40	-1 1 3	36.68
2.415	20	6 0 0	37.20
2.385	6	0 1 3	37.68
2.320	5	-1 2 2	38.78
2.294	35	0 2 2	39.24
2.287	16	-2 2 2	39.36
2.250	25	-4 1 3	40.04
2.225	18	4 2 0	40.51
2.216	16	1 2 2	40.68
2.125	12	2 1 3	42.50
2.086	12	-4 2 2	43.34
2.018	5	6 1 1	44.89
1.975	11	0 0 4	45.90
1.963M	11	3 2 2	46.21
1.963M		-4 0 4	46.21
1.941	5	-6 1 3	46.76
1.859	5	6 0 2	48.97
1.837	13	-8 0 2	49.59
1.827M	16	-1 3 1	49.87
1.827M		0 3 1	49.87
1.805	10	-6 2 2	50.52
1.789	9	7 1 1	51.00
1.785	12	-7 1 3	51.14
1.745	1	-3 3 1	52.39
1.6761	11	3 3 1	54.72
1.6727	9	-4 3 1	54.84
1.6552	7	-2 2 4	55.47
1.6175	2	0 2 4	56.88
1.5957	5	-9 1 1	57.73
1.5677	3	-3 1 5	58.86
1.5502	17	-8 0 4	59.59
1.5479	16	-4 1 5	59.69
1.5281	7	6 1 3	60.54
1.5229	10	0 1 5	60.77
1.5115M	11	-5 1 5	61.28
1.5115M		2 2 4	61.28
1.5072+	10	5 3 1	61.47
1.5072+		8 0 2	61.47
1.4980	6	1 3 3	61.89
1.4759	5	1 1 5	62.92

Zinc Phosphate, β -$Zn_3(PO_4)_2$

CAS registry no.
7779-90-0

Sample
The sample was prepared by heating $ZnCO_3$ and H_3PO_4 together at 1000 °C for several days, and cooling rapidly.

Color
Colorless

Structure
Monoclinic, $P2_1/a$ (14), Z = 4. The structure of β -$Zn_3(PO_4)_2$ was determined by Stephens and Calvo [1967].

Lattice constants of this sample
a = 8.685(2) Å
b = 9.179(1)
c = 8.265(1)
β = 112.80(1)°

a/b = 0.9462
c/b = 0.9004

Volume
607.5 $Å^3$

Density
(calculated) 4.221 g/cm^3

Figure of merit
F_{30} = 88.4(0.009,36)

Polymorphism
$Zn_3(PO_4)_2$ has an inversion from α to β form at 942 °C. This is sluggish so that the β (high) form exists metastably at room temperature. [Stephens and Calvo, 1967] [Katnack and Hummel, 1958].

Additional pattern
1. PDF card 11-27 [Katnack and Hummel, 1958]

References
Katnack, F. L. and Hummel, F. A. (1958). J. Electrochem. Soc. 105, 125.
Stephens, J. S. and Calvo, C. (1967). Can. J. Chem. 45, 2303.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
7.61	3	0 0 1	11.62
6.04	2	1 1 0	14.66
5.590	2	-1 1 1	15.84
4.296	5	-2 0 1	20.66
4.178	12	1 1 1	21.25
4.008	9	2 0 0	22.16
3.931	35	0 2 1	22.60
3.890	25	-2 1 1	22.84
3.810	3	0 0 2	23.33
3.753	2	-1 1 2	23.69
3.669	14	2 1 0	24.24
3.526	9	-2 0 2	25.24
3.290	100	-2 1 2	27.08
3.135	35	-2 2 1	28.45
3.084	45	2 0 1	28.93
3.064	55	-1 2 2	29.12
3.018	30	2 2 0	29.58
2.931	10	0 2 2	30.47
2.927	7	2 1 1	30.52
2.866	80	1 1 2	31.18
2.839	50	0 3 1	31.49
2.808	11	-1 3 1	31.84
2.759	2	-3 1 1	32.43
2.661	4	-2 0 3	33.65
2.626	4	-3 1 2	34.12
2.561+	15	1 3 1	35.01
2.561+		2 2 1	35.01
2.557	14	-2 1 3	35.06
2.539	11	0 0 3	35.32
2.491	35	-2 3 1	36.02
2.455	6	-1 3 2	36.58
2.449M	8	0 1 3	36.67
2.449M		-3 2 1	36.67
2.431	3	2 3 0	36.95
2.387	25	0 3 2	37.65
2.357	10	-1 2 3	38.15
2.352	8	-3 2 2	38.23
2.343	3	2 0 2	38.38
2.306	9	3 2 0	39.02
2.300	9	-2 2 3	39.13
2.296	11	0 4 0	39.20
2.269	3	2 1 2	39.69
2.206	6	1 4 0	40.88
2.197	14	0 4 1	41.04
2.182	5	-1 4 1	41.34
2.173	3	2 3 1	41.53
2.148M	14	1 3 2	42.02
2.148M		-4 0 2	42.02
2.128	3	1 1 3	42.44
2.103	8	-3 3 1	42.97
2.091M	18	-3 2 3	43.24
2.091M		-4 1 2	43.24
2.087	16	2 2 2	43.33
2.061	1	1 4 1	43.89
2.043M	3	-1 3 3	44.30
2.043M		-3 3 2	44.30
2.028	9	3 2 1	44.64
2.024	10	-2 4 1	44.74
2.007M	11	-2 3 3	45.14
2.007M		-2 1 4	45.14

d(Å)	I	hkℓ	2θ(°)
1.992M	8	-4 0 3	45.51
1.992M		-1 1 4	45.51
1.976	1	1 2 3	45.89
1.965	2	0 4 2	46.15
1.954M	4	4 1 0	46.43
1.954M		0 3 3	46.43
1.945M	7	-4 1 3	46.66
1.945M		-4 2 2	46.66
1.923	6	-2 4 2	47.22
1.9054M	14	-3 1 4	47.69
1.9054M		0 0 4	47.69
1.8766	7	-2 2 4	48.47
1.8657	9	0 1 4	48.77
1.8632M	25	-1 2 4	48.84
1.8632M		-3 3 3	48.84
1.8597	20	2 3 2	48.94
1.8455	3	2 0 3	49.34
1.8344M	4	4 2 0	49.66
1.8344M		3 1 2	49.66
1.8268M	5	-4 2 3	49.88
1.8268M		1 4 2	49.88
1.8098	5	2 1 3	50.38
1.7899	6	1 5 0	50.98
1.7750	9	4 0 1	51.44
1.7613+	3	-1 4 3	51.87
1.7613+		-4 3 1	51.87
1.7395	2	3 4 0	52.57
1.7096	12	1 5 1	53.56
1.7034	10	0 4 3	53.77
1.6872	10	-2 5 1	54.33
1.6772M	13	-5 1 1	54.68
1.6772M		-1 5 2	54.68
1.6699M	7	-4 3 3	54.94
1.6699M		2 5 0	54.94
1.6525M	8	-2 0 5	55.57
1.6525M		-5 1 3	55.57
1.6427M	13	-3 3 4	55.93
1.6427M		-3 4 3	55.93
1.6280	5	-2 5 2	56.48
1.6240	6	-5 2 2	56.63
1.6105	2	3 4 1	57.15
1.6023	9	1 2 4	57.47
1.5972M	6	3 3 2	57.67
1.5972M		-3 1 5	57.67
1.5924	3	-1 1 5	57.86
1.5679M	12	1 5 2	58.85
1.5679M		-4 4 2	58.85
1.5557	2	-2 2 5	59.36
1.5502	4	-3 5 1	59.59
1.5399	5	3 1 3	60.03

d(Å)	I	hkℓ	2θ(°)
1.5313M	7	-4 0 5	60.40
1.5313M		-2 4 4	60.40
1.5245+	6	-1 2 5	60.70
1.5245+		-1 4 4	60.70
1.5117+	7	5 2 0	61.27
1.5117+		-2 5 3	61.27
1.5083M	9	4 4 0	61.42
1.5083M		2 0 4	61.42
1.5041M	10	-4 4 3	61.61
1.5041M		0 1 5	61.61

Zinc Phosphate, γ-$Zn_3(PO_4)_2$

Sample
This sample was prepared by heating stoichiometric amounts of $ZnCO_3$ and H_3PO_4 with 3% of the $ZnCO_3$ replaced by $MnCO_3$, at 900 °C for several days. This phase has useful luminescence properties, and is only stabilized by the addition of low percents of certain other bivalent cations [Calvo, 1965].

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14), Z = 2. The structure of γ-$Zn_3(PO_4)_2$ was determined by Calvo [1963].

Lattice constants of this sample

a = 7.549(1) Å
b = 8.499(1)
c = 5.0491(8)
β = 95.03(1)°

a/b = 0.8882
c/b = 0.5941

Volume
322.7 Å^3

Density
(calculated) 3.973 g/cm^3

Figure of merit
F_{30} = 85.9 (0.009,37)

Reference intensity
$I/I_{corundum}$ = 1.6(2)

Polymorphism
Without the addition of other bivalent ions $Zn_3(PO_4)_2$ exists in an α form below 942 °C and in a β form above. Both are monoclinic [Calvo, 1965].

Additional pattern
1. Hummel and Katnack [1958]

References
Calvo, C. (1963). J. Phys. Chem. Solids. 24, 141.
Calvo, C. (1965). Can. J. Chem. 43, 436.
Hummel, F. A. and Katnack, F. L. (1958). J. Electrochem. Soc. 105, 528.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I	hkℓ	2θ(°)
5.626	6	1 1 0	15.74
4.363	80	-1 0 1	20.34
4.331	25	0 1 1	20.49
4.249	3	0 2 0	20.89
4.023	40	1 0 1	22.08
3.880	25	-1 1 1	22.90
3.700	6	1 2 0	24.03
3.435	100	2 1 0	25.92
3.244	20	0 2 1	27.47
3.042	19	-1 2 1	29.34
2.919	8	1 2 1	30.60
2.817	25	2 2 0	31.74
2.738	13	2 1 1	32.68
2.651	10	1 3 0	33.78
2.530	35	-2 2 1	35.45
2.515	30	0 0 2	35.67
2.468	45	0 3 1	36.37
2.404	20	3 1 0	37.38
2.391	8	2 2 1	37.59
2.376	2	-1 3 1	37.84
2.355	2	-1 1 2	38.19
2.327	2	-3 0 1	38.66
2.316	8	1 3 1	38.86
2.245	10	-3 1 1	40.14
2.181	2	-2 0 2	41.37
2.168	4	3 0 1	41.62
2.164	2	0 2 2	41.71
2.124M	13	0 4 0	42.52
2.124M		-1 2 2	42.52
2.105	20	-2 3 1	42.92
2.101	20	3 1 1	43.02
2.040M	18	-3 2 1	44.37
2.040M		1 2 2	44.37
2.012	3	2 0 2	45.03
1.9570M	2	0 4 1	46.36
1.9570M		2 1 2	46.36
1.9392	4	-2 2 2	46.81
1.9322	2	3 2 1	46.99
1.9103	4	-1 4 1	47.56
1.8799+	5	0 3 2	48.38
1.8799+		4 0 0	48.38
1.8766	4	3 3 0	48.47
1.8536	14	-1 3 2	49.11
1.8497	8	2 4 0	49.22
1.8176	7	2 2 2	50.15
1.8149	4	-3 1 2	50.23
1.7975M	4	-3 3 1	50.75
1.7975M		1 3 2	50.75
1.7743	14	-4 1 1	51.46
1.7613	4	-2 4 1	51.87

Zinc Phosphate, γ -$Zn_3(PO_4)_2$ - (continued)

d(Å)	I	hkℓ	2θ(°)
1.7197	2	4 2 0	53.22
1.7029	6	-3 2 2	53.79
1.6792	6	4 1 1	54.61
1.6691M	12	3 1 2	54.97
1.6691M		-4 2 1	54.97
1.6579	6	1 5 0	55.37
1.6368	5	-1 1 3	56.15
1.6063M	2	1 0 3	57.31
1.6063M		-1 4 2	57.31
1.5881	1	4 2 1	58.03
1.5667M	5	4 3 0	58.90
1.5667M		1 5 1	58.90
1.5595	10	0 2 3	59.20
1.5545	12	-3 3 2	59.41
1.5493	10	2 5 0	59.63

Zinc Phosphate Hydrate (Hopeite), $Zn_3(PO_4)_2 \cdot 4H_2O$

CAS registry no.
7543-51-3

Sample
The sample was a reagent from the Chicago Apparatus Co., recrystallized from aqueous solution.

Color
Colorless

Structure
Orthorhombic, Pnma (62), Z = 4. The structure of hopeite has been determined by Mamedov et al. [1961] and Liebau [1965].

Lattice constants of this sample
a = 10.611(1) Å
b = 18.312(2)
c = 5.0309(6)

a/b = 0.5795
c/b = 0.2747

Volume
977.55 Å^3

Density
(calculated) 3.113 g/cm^3

Figure of merit
F_{30} = 73.8(0.010,40)

Polymorphism
A polymorph of $Zn_3(PO_4)_2 \cdot 4H_2O$ is called parahopeite [Chao, 1969]. The pattern for parahopeite is on card 24-1461.

Additional patterns
1. PDF card 1-964 [Hanawalt et al., 1938]
2. PDF card 9-497 [Murdoch, Univ. of Cal., Los Angeles, Calif.], natural mineral.
3. PDF card 23-747 [Komrska and Satava 1969]
4. PDF card 26-1397 [Whitaker, 1973], natural mineral

References

Chao, G. Y. (1969). Z. Kristallogr, Kristallgeometrie Kristallphys. Kristallchem. 130, 261.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Komrska, J. and Satava, V. (1969). Silikaty 13, 135.
Liebau, F. (1965). Acta Crystallogr. 18, 352.
Mamedov, C. S., Gamidov, R., and Belov, N. W. (1961). Kristallographia 6, 114.
Whitaker, A., (1973). J. Appl. Crystallogr. 6, 495.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I	hkℓ	2θ(°)
9.16	55	0 2 0	9.65
5.311	17	2 0 0	16.68
5.095	25	2 1 0	17.39
4.855	30	0 1 1	18.26
4.576	55	0 4 0	19.38
4.414	35	1 1 1	20.10
4.072	7	1 2 1	21.81
4.005	20	2 3 0	22.18
3.880	14	0 3 1	22.90
3.648M	9	2 0 1	24.38
3.648M		1 3 1	24.38
3.468	30	2 4 0	25.67
3.391	40	2 2 1	26.26
3.225	1	1 4 1	27.64
3.134	9	2 3 1	28.46
3.053	1	0 6 0	29.23
3.015	4	2 5 0	29.61
2.963	8	0 5 1	30.14
2.855+	100	3 1 1	31.30
2.855+		2 4 1	31.30
2.760	3	3 2 1	32.41
2.652	19	4 0 0	33.77
2.614	25	3 3 1	34.28
2.585	3	2 5 1	34.67
2.548	15	4 2 0	35.19
2.535	11	1 6 1	35.38
2.515	15	0 0 2	35.67
2.445M	3	1 0 2	36.72
2.445M		3 4 1	36.72
2.426M	10	1 1 2	37.02
2.426M		0 2 2	37.02
2.342	7	2 6 1	38.40
2.321	1	0 7 1	38.77
2.288	7	0 8 0	39.35
2.271M	15	1 3 2	39.66
2.271M		3 5 1	39.66
2.268	13	1 7 1	39.71
2.206M	4	2 2 2	40.88
2.206M		0 4 2	40.88
2.190	2	4 3 1	41.18
2.158	7	1 4 2	41.83
2.148	3	4 5 0	42.02
2.130	1	2 3 2	42.41
2.100M	11	2 8 0	43.03
2.100M		3 6 1	43.03
2.038M	3	3 1 2	44.42
2.038M		2 4 2	44.42
2.002M	16	4 6 0	45.26
2.002M		3 2 2	45.26
1.977	2	4 5 1	45.87

d(Å)	I	hkℓ	2θ(°)
1.940+	25	3 7 1	46.79
1.940+		2 8 1	46.79
1.9111	2	5 2 1	47.54
1.8994	1	2 9 0	47.85
1.8715	1	3 4 2	48.61
1.8618M	2	4 7 0	48.88
1.8618M		5 3 1	48.88
1.8247	15	4 0 2	49.94
1.7985	1	5 4 1	50.72
1.7896M	1	4 2 2	50.99
1.7896M		3 5 2	50.99
1.7772	3	2 9 1	51.37
1.7361	5	6 2 0	52.68
1.7306	4	2 10 0	52.86
1.7252	3	5 5 1	53.04
1.7014	2	3 6 2	53.84
1.6953	6	4 4 2	54.05
1.6719	6	1 8 2	54.87
1.6646	5	3 9 1	55.13
1.6370	5	2 10 1	56.14
1.6298	3	1 2 3	56.41
1.6169	3	0 3 3	56.90
1.6143M	4	4 9 0	57.00
1.6143M		3 7 2	57.00
1.5974	4	5 2 2	57.66
1.5931M	4	2 1 3	57.83
1.5931M		6 5 0	57.83
1.5755M	1	2 2 3	58.54
1.5672+	10	5 3 2	58.88
1.5672+		6 4 1	58.88
1.5633	9	1 11 1	59.04
1.5295M	9	6 6 0	60.48
1.5295M		5 4 2	60.48
1.5254M	10	0 12 0	60.66
1.5254M		0 5 3	60.66
1.5161M	3	2 9 2	61.07
1.5161M		3 0 3	61.07
1.5092M	10	2 4 3	61.38
1.5092M		1 5 3	61.38
1.5068	7	4 10 0	61.49

Aluminum Iron Antimony Oxide, Bahianite, $Al_{5.66}Fe_{0.09}Sb_{2.95}O_{16}$

Structure

Monoclinic, C2/m (12), Z = 2. The structure was determined by Moore and Araki [1976], for a sample from Serra de Mangabeira, Bahia, Brazil.

Atom positions

2(a)	1.8 antimony and 0.2 iron
4(g)	4 antimony
2(d)	2 aluminum
8(j)	7.52 aluminum and 0.48 iron
8(j)	8 oxygen in each of 3 different sites
4(i)	4 oxygen in each of 2 different sites

The single crystal analysis did not refine positions for the Al atoms in the tetrahedral sites and they were omitted also from calculation of this powder pattern. Minor amounts of W^{+6} in the octahedral sites were not determined either but their contribution was absorbed into the site distribution refinement [Moore and Araki, 1976].

Lattice constants

$a = 9.407(6)$ Å
$b = 11.542(8)$
$c = 4.410(3)$
$\beta = 90.94(3)°$

$a/b = 0.8150$
$c/b = 0.3821$

(published values: $a = 9.406(6)$ Å, $b = 11.541(8)$, $c = 4.410(3)$, $\beta = 90.94(3)°$ [Moore and Araki, 1976]).

Volume

478.75 Å^3

Density

(calculated) 5.362 g/cm^3

This is the value calculated from the formula above, based on a chemical analysis by Moore and Araki in their table 1 part A [1976]. Due to the problems in the site distribution, mentioned above, a density is different if calculated from the multiplicities given in the atom positions.

Thermal parameters

Isotropic [Moore and Araki, 1976]

Scattering factors

Al^{3+}, Fe^{3+}, O^{1-}, Sb^{5+} [Cromer and Mann, 1968]. Dispersion corrections were applied to Al, Fe, and O [Cromer and Liberman, 1970].

Scale factors (integrated intensities)

$\gamma = 0.1911 \times 10^{-3}$

$I/I_{corundum}$ (calculated) = 1.74 for reflection with hkℓ = $\bar{2}01$

References

Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.

Cromer, D. T. and Liberman, D. J. (1970). J. Chem. Phys. 53, 1891.

Moore, P. B. and Araki, T. (1976). Neues Jahrb. Mineral. Abh. 126, 113.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
7.28	27	1 1 0	12.14
5.76	18	0 2 0	15.36
4.70	84	2 0 0	18.86
4.41	40	0 0 1	20.14
3.792	21	-1 1 1	23.44
3.751	18	1 1 1	23.70
3.645	10	2 2 0	24.40
3.559	30	1 3 0	25.00
3.504	25	0 2 1	25.40
3.243	100	-2 0 1	27.48
3.191	99	2 0 1	27.94
3.026	2	3 1 0	29.50
2.884	21	0 4 0	30.98
2.827	17	-2 2 1	31.62
2.778	37	-1 3 1	32.20
2.763	33	1 3 1	32.38
2.513	10	-3 1 1	35.70
2.4755	10	3 1 1	36.26
2.4597	53	2 4 0	36.50
2.4302	19	3 3 0	36.96
2.4138	57	0 4 1	37.22
2.3517	21	4 0 0	38.24
2.2047	11	0 0 2	40.90
2.1772	5	4 2 0	41.44
2.1553	49	-2 4 1	41.88
2.1397	19	-3 3 1	42.20
2.1168	10	3 3 1	42.68
2.1027	3	1 1 2	42.98
2.0607	24	4 0 1	43.90
2.0087	5	-2 0 2	45.10
1.9837	13	2 0 2	45.70
1.9642	4	-4 2 1	46.18
1.9404	4	4 2 1	46.78
1.8968	2	-2 2 2	47.92
1.8799	7	-1 3 2	48.38
1.8755	6	2 2 2	48.50
1.8697	5	1 3 2	48.66
1.8568	2	5 1 0	49.02
1.8227	11	4 4 0	50.00
1.7802	1	2 6 0	51.28
1.7629	2	0 6 1	51.82
1.7515	9	0 4 2	52.18
1.7209	1	-5 1 1	53.18
1.6921	24	-4 4 1	54.16
1.6772	23	4 4 1	54.68

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.6489	34	-2 4 2	55.70
1.6349	37	2 4 2	56.22
1.6216	31	-4 0 2+	56.72
1.5954	17	4 0 2	57.74
1.5859	8	-5 3 1	58.12
1.5701	9	5 3 1	58.76
1.5672	8	6 0 0	58.88
1.5378	1	4 2 2	60.12
1.5254	10	-1 7 1	60.66
1.5222	13	1 7 1	60.80
1.5132	1	6 2 0	61.20
1.4848	7	-6 0 1	62.50
1.4697	8	6 0 1+	63.22
1.4593	5	3 7 0+	63.72
1.4428	12	0 8 0	64.54

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
7.29	23	1 1 0	12.13
5.77	16	0 2 0	15.34
4.70	78	2 0 0	18.85
4.41	38	0 0 1	20.12
3.795	20	-1 1 1	23.43
3.752	16	1 1 1	23.69
3.646	9	2 2 0	24.40
3.561	29	1 3 0	24.99
3.504	24	0 2 1	25.40
3.243	100	-2 0 1	27.48
3.191	100	2 0 1	27.94
3.026	2	3 1 0	29.50
2.885	21	0 4 0	30.97
2.827	17	-2 2 1	31.62
2.792	14	2 2 1	32.03
2.779	33	-1 3 1	32.19
2.762	29	1 3 1	32.39
2.513	10	-3 1 1	35.69
2.4765	7	3 1 1	36.24
2.4595	57	2 4 0	36.50
2.4304	15	3 3 0	36.96
2.4145	61	0 4 1	37.21
2.3514	23	4 0 0	38.24
2.2047	12	0 0 2	40.90
2.1776	3	4 2 0	41.43
2.1558	54	-2 4 1	41.87
2.1401	1	2 4 1	42.19
2.1400	17	-3 3 1	42.19
2.1178	1	-1 1 2	42.66
2.1172	10	3 3 1	42.67
2.1029	2	1 1 2	42.97
2.0609	24	4 0 1	43.90
2.0595	3	0 2 2	43.93
2.0089	5	-2 0 2	45.09
1.9838	14	2 0 2	45.70
1.9644	5	-4 2 1	46.17
1.9408	4	4 2 1	46.77
1.8973	2	-2 2 2	47.91
1.8797	7	-1 3 2	48.38
1.8760	1	2 2 2	48.49
1.8693	5	1 3 2	48.67
1.8566	1	5 1 0	49.02
1.8228	13	4 4 0	50.00
1.7805	1	2 6 0	51.27
1.7632	2	0 6 1	51.81
1.7519	10	0 4 2	52.17
1.7211	1	-5 1 1	53.17
1.7013	1	5 1 1	53.84
1.6922	26	-4 4 1	54.16
1.6900	3	5 3 0	54.23
1.6770	26	4 4 1	54.69
1.6487	38	-2 4 2	55.71
1.6474	1	2 6 1	55.75
1.6434	5	-3 3 2	55.90
1.6347	42	2 4 2	56.23
1.6241	12	1 7 0	56.63
1.6227	5	3 3 2	56.68
1.6217	25	-4 0 2	56.72
1.5953	20	4 0 2	57.74
1.5859	8	-5 3 1	58.12
1.5703	9	5 3 1	58.75
1.5689	1	1 5 2	58.81
1.5676	5	6 0 0	58.86
1.5612	1	-4 2 2	59.13
1.5377	1	4 2 2	60.13
1.5254	10	-1 7 1	60.66
1.5226	10	1 7 1	60.78
1.5128	1	6 2 0	61.22
1.4848	8	-6 0 1	62.50
1.4698	3	0 0 3	63.21
1.4695	6	6 0 1	63.23
1.4593	5	3 7 0	63.72
1.4583	1	5 5 0	63.77
1.4444	1	-1 1 3	64.46
1.4427	14	0 8 0	64.54
1.4379	2	-6 2 1	64.78

Antimony Iron Titanium Oxide Hydroxide, Derbylite, $SbFe_4Ti_3O_{13}(OH)$

Structure
Monoclinic, $P2_1/m$ (11), Z = 2. The structure was determined by Moore and Araki [1976] using data from sample #C4430, U.S. National Museum. The original location was Diamantina, Minas Gerais, Brazil.

Atom positions
Moore and Araki [1976]

2(e)	2 antimony
2(e)	2 titanium
4(f)	1.72 iron and 2.28 titanium
4(f)	1.72 titanium and 2.28 iron
2(e)	2 oxygen
2(e)	2 hydroxyl
4(f)	4 oxygen in each of 6 different sites
4(f)	4 iron

Lattice constants
a = 7.160(1) Å
b = 14.348(3)
c = 4.970(1)
β = 104.61(2)°

a/b = 0.4990
c/b = 0.3464

(published values: a = 7.160(1) Å, b = 14.347(3), c = 4.970(1), β = 104.61(2)° [Moore and Araki, 1976]).

Volume
494.1 $Å^3$

Density
(calculated) 4.798 g/cm^3

Thermal parameters
Isotropic [Moore and Araki, 1976]

Scattering factors
Sb^{3+}, Fe^{3+}, Ti^{4+}, O^- [Cromer and Mann, 1968]. Antimony, iron and titanium factors were corrected for dispersion [Cromer and Liberman, 1970].

Scale factors (integrated intensities)
$\gamma = 0.1340 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 1.58 for reflection with hkℓ = 131.

References

Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.
Moore, P. B. and Araki, T. (1976). Neues Jahrb. Mineral. Abh. 126, 292.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
6.23	21	1 1 0	14.20
4.98	5	1 2 0	17.80
4.81	21	0 0 1	18.44
4.52	18	-1 0 1	19.64
4.31	5	-1 1 1	20.60
3.994	26	0 2 1	22.24
3.935	7	1 3 0	22.58
3.824	25	-1 2 1	23.24
3.584	3	0 4 0	24.82
3.553	5	1 0 1	25.04
3.461	4	2 0 0	25.72
3.453	4	1 1 1	25.78
3.366	16	2 1 0	26.46
3.222	8	-2 0 1	27.66
3.184	37	1 4 0+	28.00
3.119	50	2 2 0	28.60
2.940	10	-2 2 1	30.38
2.852	100	1 3 1	31.34
2.808	19	-1 4 1+	31.84
2.673	90	-2 3 1	33.50
2.524	4	1 4 1	35.54
2.486	13	2 1 1	36.10
2.473	34	-1 0 2	36.30
2.468	29	0 5 1	36.38
2.423	5	-1 5 1	37.08
2.391	16	0 6 0	37.58
2.372	4	0 1 2	37.90
2.338	2	-1 2 2	38.48
2.309	3	3 0 0	38.98
2.293	8	-3 1 1	39.26
2.280	8	3 1 0+	39.50
2.260	6	1 6 0	39.86
2.232	21	1 5 1	40.38
2.210	5	2 5 0+	40.80
2.199	3	3 2 0	41.02
2.143	13	-2 5 1+	42.14
2.113	7	1 0 2+	42.76
2.090	7	1 1 2+	43.26
2.080	5	3 3 0	43.48
2.027	15	1 2 2	44.68
1.997	8	0 4 2	45.38
1.984	2	1 6 1	45.70
1.966	2	1 7 0	46.14
1.942	2	3 4 0	46.74
1.932	3	1 3 2	47.00
1.926	8	-3 0 2	47.16
1.921	7	-2 6 1	47.28
1.913	9	-2 4 2+	47.50
1.8953	3	2 5 1	47.96
1.8865	6	3 1 1+	48.20

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.8604	9	-3 2 2	48.92
1.8427	2	0 5 2	49.42
1.8051	5	-3 5 1	50.52
1.7998	6	3 5 0	50.68
1.7763	15	2 0 2+	51.40
1.7641	8	-4 1 1+	51.78
1.7361	3	1 8 0	52.68
1.7294	5	-2 7 1	52.90
1.7246	5	2 2 2	53.06
1.7191	16	-1 6 2+	53.24
1.7014	2	1 5 2	53.84
1.6967	2	0 6 2	54.00
1.6806	2	0 8 1	54.56
1.6665	6	2 3 2+	55.06
1.6615	7	3 6 0	55.24
1.6571	4	-1 0 3	55.40
1.6424	6	-2 6 2	55.94
1.6285	2	4 3 0	56.46
1.6112	10	-4 0 2	57.12
1.6010	4	-4 1 2+	57.52
1.5924	17	2 8 0	57.86
1.5859	28	3 5 1	58.12
1.5721	3	-4 2 2	58.68
1.5672	3	-2 8 1	58.88
1.5648	4	-1 3 3+	58.98
1.5600	4	4 4 0+	59.18
1.5369	4	-3 7 1	60.16
1.5332	5	-2 3 3+	60.32
1.5272	3	-4 3 2	60.58
1.5200	12	0 3 3	60.90
1.5119	20	-4 5 1+	61.26
1.5039	6	4 1 1+	61.62
1.5004	4	-3 6 2+	61.78
1.4887	3	3 0 2	62.32
1.4831	2	4 5 0	62.58
1.4802	2	4 2 1+	62.72
1.4743	6	1 1 3+	63.00
1.4709	5	1 7 2+	63.16
1.4544	2	1 9 1	63.96
1.4420	3	4 3 1	64.58
1.4344	24	-1 5 3+	64.96
1.4239	5	-5 1 1	65.50
1.4208	3	3 3 2	65.66
1.4098	2	-2 5 3	66.24
1.4049	5	-2 8 2+	66.50
1.4015	3	0 5 3	66.68

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
6.24	18	1 1 0	14.18
4.98	4	1 2 0	17.78
4.81	18	0 0 1	18.43
4.52	16	-1 0 1	19.62
4.31	4	-1 1 1	20.58
3.995	24	0 2 1	22.24
3.936	6	1 3 0	22.57
3.825	24	-1 2 1	23.24
3.587	3	0 4 0	24.80
3.553	4	1 0 1	25.04
3.464	3	2 0 0	25.70
3.449	2	1 1 1	25.81
3.391	3	0 3 1	26.26
3.367	15	2 1 0	26.45
3.223	6	-2 0 1	27.66
3.185	26	1 4 0	27.99
3.184	10	1 2 1	28.00
3.120	49	2 2 0	28.59
2.940	10	-2 2 1	30.38
2.875	11	0 4 1	31.08
2.852	100	1 3 1	31.34
2.810	14	-1 4 1	31.82
2.806	4	2 3 0	31.87
2.673	94	-2 3 1	33.50
2.651	2	1 5 0	33.78
2.524	4	1 4 1	35.53
2.487	10	2 1 1	36.09
2.473	32	-1 0 2	36.30
2.464	11	0 5 1	36.43
2.423	5	-1 5 1	37.08
2.397	4	-2 4 1	37.49
2.391	14	0 6 0	37.58
2.372	3	0 1 2	37.91
2.338	2	-1 2 2	38.47
2.309	3	3 0 0	38.97
2.293	8	-3 1 1	39.26
2.280	6	3 1 0	39.49
2.280	2	0 2 2	39.49
2.260	5	1 6 0	39.85
2.260	1	-2 0 2	39.85
2.232	22	1 5 1	40.37
2.210	1	-3 2 1	40.80
2.210	3	2 5 0	40.80
2.198	2	3 2 0	41.02
2.148	2	0 3 2	42.02
2.143	10	-2 5 1	42.13
2.141	3	0 6 1	42.17
2.114	3	-1 6 1	42.74
2.113	4	1 0 2	42.77
2.090	4	1 1 2	43.25

d(Å)	I	hkℓ	2Θ(°) λ - 1.540598Å
2.090	3	-3 3 1	43.26
2.080	4	3 3 0	43.48
2.036	1	-1 4 2	44.46
2.027	17	1 2 2	44.68
1.997	8	0 4 2	45.37
1.984	2	1 6 1	45.69
1.966	2	1 7 0	46.15
1.942	1	3 4 0	46.74
1.932	2	1 3 2	46.98
1.926	8	-3 0 2	47.15
1.920	2	-2 6 1	47.30
1.912	8	-2 4 2	47.51
1.909	3	-3 1 2	47.60
1.8957	2	2 5 1	47.95
1.8865	5	3 1 1	48.20
1.8856	2	0 7 1	48.22
1.8668	1	-1 7 1	48.74
1.8601	9	-3 2 2	48.93
1.8431	1	0 5 2	49.41
1.8056	5	-3 5 1	50.51
1.7992	5	3 5 0	50.70
1.7766	14	2 0 2	51.39
1.7755	3	1 7 1	51.42
1.7682	1	3 3 1	51.65
1.7655	4	-4 1 1	51.74
1.7641	2	2 7 0	51.78
1.7631	3	2 1 2	51.81
1.7363	3	1 8 0	52.67
1.7321	1	4 0 0	52.81
1.7295	4	-2 7 1	52.90
1.7245	1	2 2 2	53.06
1.7196	2	4 1 0	53.22
1.7191	15	-1 6 2	53.24
1.7013	2	1 5 2	53.84
1.6956	1	0 6 2	54.04
1.6805	2	0 8 1	54.57
1.6674	2	-4 3 1	55.03
1.6671	2	-1 8 1	55.04
1.6654	2	2 3 2	55.10
1.6612	5	3 6 0	55.25
1.6563	1	-1 0 3	55.43
1.6427	7	-2 6 2	55.93
1.6286	1	4 3 0	56.46
1.6138	1	-1 2 3	57.02
1.6114	10	-4 0 2	57.11
1.6013	2	-4 1 2	57.51
1.6011	1	1 8 1	57.52
1.5927	17	2 8 0	57.85
1.5914	1	2 7 1	57.90
1.5859	29	3 5 1	58.12

d(Å)	I	hkℓ	2Θ(°) λ - 1.540598Å
1.5791	2	-2 2 3	58.39
1.5722	2	-4 2 2	58.67
1.5672	2	-2 8 1	58.88
1.5651	2	-1 3 3	58.97
1.5599	1	0 7 2	59.18
1.5598	1	4 4 0	59.19
1.5370	4	-3 7 1	60.16
1.5333	2	-2 3 3	60.31
1.5330	1	3 7 0	60.33
1.5270	1	-4 3 2	60.59
1.5200	13	0 3 3	60.90
1.5132	2	0 9 1	61.20
1.5120	20	-4 5 1	61.26
1.5105	2	2 5 2	61.32
1.5042	2	4 1 1	61.61
1.5037	1	-1 4 3	61.63
1.5035	1	-1 9 1	61.64
1.4886	3	3 0 2	62.32
1.4829	1	4 5 0	62.59
1.4800	1	4 2 1	62.73
1.4755	3	-2 4 3	62.94
1.4748	1	-3 2 3	62.98
1.4741	4	1 1 3	63.01
1.4711	1	1 7 2	63.15
1.4699	1	-4 4 2	63.21
1.4545	1	1 9 1	63.96
1.4519	1	-1 8 2	64.08
1.4421	2	4 3 1	64.57
1.4373	9	-3 3 3	64.81
1.4348	11	0 10 0	64.94
1.4345	14	-1 5 3	64.96
1.4261	1	2 6 2	65.39
1.4240	4	-5 1 1	65.50
1.4214	1	3 3 2	65.63
1.4099	2	-2 5 3	66.23
1.4050	2	-4 5 2	66.49
1.4050	2	-2 8 2	66.50
1.4036	1	-3 7 2	66.57
1.3995	1	0 5 3	66.79

Benactyzine Hydrochloride, $C_{20}H_{26}ClNO_3$

Synonym
1. 2-Diethylaminoethyl benzilate hydrochloride

Structure
Triclinic, $P\bar{1}$ (2), Z = 2. The structure was refined by Petcher et al. [1974].

Atom positions
All atoms were in general positions 2(i).

Lattice constants
a = 8.792(4) Å
b = 15.949(8)
c = 7.091(6)
α = 95.73(1)°
β = 94.10(1)
γ = 87.57(1)

a/b = 0.5513
c/b = 0.4446

(published values: a = 879.1(4) pm, b = 1594.8(8), c = 709.1(6), α = 95.73(1)°, β = 94.10(1), γ = 87.57(1) [Petcher et al., 1974])

Volume
986.2 Å^3

Density
(calculated) 1.225 g/cm^3

Thermal parameters
Isotropic. For hydrogen atoms, overall B = 5.5. For all other atoms, isotropic B_i were estimated from β_{ij} for individual atoms.

Scattering factors
Zero ionization [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.3987 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 0.380 for reflection with hkℓ = 100.

Additional pattern
1. Folen [1975]

References
Folen, V. A. (1975). J. Forensic Sci. 20, 348.
International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.
Petcher, T. J., Ramsay, W., and Forster, R. (1974). J. Chem. Soc. Perkin II, 1151.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
15.83	40	0 1 0	5.58
8.75	60	1 0 0	10.10
7.91	4	0 2 0	11.18
7.78	13	1 1 0	11.36
7.56	14	-1 1 0	11.70
7.03	8	0 0 1	12.58
6.67	39	0 -1 1	13.26
6.21	3	0 1 1	14.26
5.77	48	-1 2 0	15.34
5.53	100	0 -2 1+	16.02
5.29	14	0 3 0	16.76
5.02	2	0 2 1	17.64
4.96	1	1 1 1	17.86
4.85	4	-1 -2 1	18.26
4.52	2	1 -2 1	19.62
4.454	7	-1 3 0	19.92
4.410	7	-1 2 1	20.12
4.312	24	1 2 1	20.58
4.263	10	2 1 0	20.82
4.184	2	-2 1 0	21.22
4.081	4	-1 -3 1	21.76
4.044	1	0 3 1	21.96
3.962	3	0 4 0	22.42
3.890	3	2 2 0	22.84
3.844	8	1 -3 1	23.12
3.776	43	-2 2 0	23.54
3.657	37	1 4 0+	24.32
3.610	6	2 0 1+	24.64
3.573	6	-2 -2 1	24.90
3.509	26	0 -1 2+	25.36
3.432	6	2 3 0	25.94
3.341	21	-2 2 1+	26.66
3.314	19	0 4 1+	26.88
3.262	3	2 2 1	27.32
3.236	3	-2 -3 1	27.54
3.204	9	-1 -2 2+	27.82
3.175	4	1 -1 2	28.08
3.102	11	1 4 1+	28.76
3.010	8	2 -3 1	29.66
3.006	8	0 -5 1	29.70
2.974	1	-1 -3 2+	30.02
2.921	1	3 0 0	30.58
2.888	4	3 1 0+	30.94
2.854	4	-3 1 0	31.32
2.807	2	0 3 2	31.86
2.764	4	-3 0 1+	32.36
2.746	12	-2 1 2	32.58
2.701	2	-1 -4 2+	33.14
2.670	3	-3 -2 1	33.54
2.665	3	1 5 1+	33.60

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.644	3	2 4 1+	33.88
2.614	3	2 5 0	34.28
2.598	3	2 1 2+	34.50
2.583	6	1 -4 2	34.70
2.553	3	-3 2 1+	35.12
2.527	2	-2 5 0	35.50
2.505	3	-1 6 0+	35.82
2.481	2	2 2 2+	36.18
2.433	1	-1 -5 2+	36.92
2.399	3	0 6 1+	37.46
2.393	3	3 4 0	37.56
2.362	3	3 -3 1	38.06
2.355	3	0 -1 3+	38.18
2.349	3	-2 5 1+	38.28
2.340	2	1 -5 2	38.44
2.326	2	2 3 2+	38.68
2.312	3	-3 4 0	38.92
2.300	2	2 6 0	39.14
2.263	1	2 -4 2+	39.80
2.229	1	1 0 3+	40.44
2.221	1	0 -7 1+	40.58
2.213	1	1 7 0	40.74
2.190	3	4 0 0+	41.18
2.181	4	-1 -7 1+	41.36
2.170	3	1 5 2	41.58
2.154	1	2 -6 1+	41.90
2.140	1	-2 -1 3	42.20
2.132	2	4 2 0+	42.36
2.112	2	-3 5 0+	42.78
2.101	1	1 2 3+	43.02
2.094	1	-4 2 0+	43.16
2.060	2	-3 3 2	43.92
2.041	2	2 7 0+	44.34
2.037	2	3 -3 2+	44.44
2.033	2	3 -5 1	44.54
2.023	2	3 5 1+	44.76
2.017	2	1 -4 3+	44.90
2.014	1	2 -1 3+	44.98
1.995	1	1 3 3+	45.42
1.987	2	2 5 2+	45.62
1.975	1	-1 -7 2+	45.90
1.965	2	-3 -5 2+	46.16
1.924	1	2 -3 3+	47.20
1.919	1	1 -7 2+	47.34
1.901	3	2 7 1+	47.80
1.830	2	-4 4 1+	49.78
1.826	2	1 8 1+	49.90
1.820	1	4 -4 1	50.08
1.804	2	0 5 3+	50.56
1.800	2	-3 2 3	50.66

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.768	1	2 -7 2+	51.66
1.760	2	0 0 4+	51.92
1.757	2	-4 3 2+	52.00
1.750	2	0 -9 1+	52.22
1.723	1	2 8 1+	53.10
1.714	1	-4 -6 1+	53.40
1.709	1	3 -6 2+	53.58
1.699	1	1 -9 1+	53.92
1.655	1	-4 -2 3+	55.48
1.619	1	-3 -6 3+	56.84
1.584	1	4 -5 2+	58.20

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
15.86	66	0 1 0	5.57
8.76	100	1 0 0	10.08
7.93	4	0 2 0	11.15
7.79	20	1 1 0	11.35
7.56	23	-1 1 0	11.70
7.04	13	0 0 1	12.56
6.68	66	0 -1 1	13.25
6.21	5	0 1 1	14.24
5.78	83	-1 2 0	15.32
5.68	1	-1 0 1	15.59
5.54	94	0 -2 1	15.99
5.53	87	-1 -1 1	16.02
5.29	24	0 3 0	16.76
5.03	3	0 2 1	17.63
4.96	1	1 1 1	17.86
4.86	6	-1 -2 1	18.25
4.52	2	1 -2 1	19.60
4.457	11	-1 3 0	19.90
4.410	11	-1 2 1	20.12
4.313	43	1 2 1	20.58
4.263	14	2 1 0	20.82
4.186	2	-2 1 0	21.21
4.081	7	-1 -3 1	21.76
4.043	1	0 3 1	21.97
3.965	5	0 4 0	22.41
3.894	4	2 2 0	22.82
3.849	11	1 -3 1	23.09
3.838	3	-2 0 1	23.15
3.805	6	-2 -1 1	23.36
3.779	80	-2 2 0	23.52
3.687	21	-1 3 1	24.12
3.662	36	1 4 0	24.29
3.661	9	-2 1 1	24.29
3.655	27	1 3 1	24.33
3.612	4	2 0 1	24.63

Benactyzine Hydrochloride, $C_{20}H_{26}ClNO_3$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
3.608	4	0 -4 1	24.66
3.575	8	-2 -2 1	24.89
3.565	1	-1 4 0	24.96
3.520	21	0 0 2	25.28
3.509	33	0 -1 2	25.36
3.434	9	2 3 0	25.92
3.418	1	-1 -4 1	26.05
3.368	15	0 1 2	26.45
3.346	20	-2 2 1	26.62
3.346	6	-1 -1 2	26.62
3.340	13	0 -2 2	26.67
3.319	16	0 4 1	26.84
3.316	5	-2 3 0	26.86
3.313	14	2 -2 1	26.89
3.262	3	2 2 1	27.32
3.238	4	-2 -3 1	27.52
3.206	9	-1 -2 2	27.80
3.205	7	-1 1 2	27.81
3.192	1	1 0 2	27.93
3.176	5	1 -1 2	28.07
3.107	2	0 2 2	28.71
3.106	4	-1 4 1	28.71
3.102	16	1 4 1	28.76
3.011	13	2 -3 1	29.64
3.003	6	0 -5 1	29.72
2.993	1	2 4 0	29.82
2.973	1	-1 -3 2	30.04
2.921	1	3 0 0	30.58
2.891	4	3 1 0	30.90
2.887	3	1 2 2	30.95
2.882	1	-2 -4 1	31.01
2.855	8	-3 1 0	31.31
2.846	2	-2 -1 2	31.41
2.807	3	0 3 2	31.86
2.792	1	0 5 1	32.03
2.769	2	0 -4 2	32.30
2.765	4	-3 0 1	32.35
2.747	24	-2 1 2	32.57
2.702	2	-1 -4 2	33.13
2.698	1	2 -4 1	33.18
2.671	4	-3 -2 1	33.52
2.664	2	1 5 1	33.62
2.658	1	2 0 2	33.70
2.649	1	-2 4 1	33.81
2.643	2	2 4 1	33.89
2.636	2	3 0 1	33.98
2.614	5	2 5 0	34.28
2.599	2	2 1 2	34.48
2.598	1	3 1 1	34.49
2.596	1	3 3 0	34.52

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.583	11	1 -4 2	34.70
2.556	1	1 6 0	35.08
2.555	2	-3 2 1	35.10
2.553	2	-2 -5 1	35.13
2.527	3	-2 5 0	35.49
2.506	5	-1 6 0	35.80
2.504	1	3 -2 1	35.83
2.498	1	3 2 1	35.92
2.482	2	2 2 2	36.17
2.479	1	0 -5 2	36.21
2.434	1	-1 -5 2	36.90
2.433	1	-1 4 2	36.92
2.408	2	2 -5 1	37.31
2.400	2	1 4 2	37.44
2.399	2	0 6 1	37.46
2.393	4	3 4 0	37.56
2.381	1	-3 3 1	37.75
2.363	4	3 -3 1	38.05
2.355	1	3 3 1	38.19
2.355	2	0 -1 3	38.19
2.350	2	-2 5 1	38.27
2.346	1	0 0 3	38.33
2.340	2	1 -5 2	38.44
2.327	2	2 3 2	38.67
2.327	1	-3 0 2	38.67
2.313	5	-3 4 0	38.91
2.300	3	2 6 0	39.14
2.262	1	2 -4 2	39.81
2.229	2	1 0 3	40.43
2.220	1	0 -7 1	40.60
2.213	2	1 7 0	40.75
2.193	2	0 2 3	41.13
2.191	2	4 0 0	41.17
2.189	2	-1 5 2	41.21
2.182	3	-1 -7 1	41.35
2.181	2	4 1 0	41.37
2.179	1	-3 2 2	41.41
2.175	1	-1 7 0	41.49
2.170	4	1 5 2	41.58
2.166	1	3 -1 2	41.66
2.154	1	2 -6 1	41.90
2.140	1	-2 -1 3	42.19
2.133	2	-4 0 1	42.33
2.131	2	4 2 0	42.37
2.113	1	-2 -2 3	42.76
2.112	1	-3 5 0	42.79
2.101	1	1 2 3	43.02
2.060	3	-3 3 2	43.91
2.046	1	1 7 1	44.23
2.042	2	2 7 0	44.32

Benactyzine Hydrochloride, $C_{20}H_{26}ClNO_3$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.037	2	3 -3 2	44.44
2.035	1	4 -1 1	44.49
2.032	1	3 -5 1	44.56
2.023	2	3 5 1	44.76
2.014	1	2 -1 3	44.98
2.013	1	2 0 3	45.01
2.004	1	-2 2 3	45.20
1.995	1	1 3 3	45.41
1.989	1	3 3 2	45.56
1.987	3	2 5 2	45.62
1.976	1	-1 -7 2	45.90
1.965	2	-3 -5 2	46.17
1.965	1	1 6 2	46.17
1.924	1	2 -3 3	47.19
1.919	1	-1 8 0	47.33
1.917	1	1 -7 2	47.39
1.907	1	-2 3 3	47.66
1.902	1	-4 -2 2	47.77
1.902	4	2 7 1	47.79
1.900	2	1 -5 3	47.84
1.830	3	-4 4 1	49.77
1.819	1	4 -4 1	50.10
1.806	1	4 0 2	50.49
1.804	1	0 5 3	50.54
1.804	1	0 -8 2	50.56
1.800	2	-3 2 3	50.66
1.770	1	2 -7 2	51.59
1.768	1	0 -1 4	51.66
1.760	2	0 0 4	51.92
1.757	1	-4 3 2	52.00
1.750	1	0 -9 1	52.23
1.735	1	-5 1 0	52.70
1.699	1	1 -9 1	53.92
1.619	1	-3 -6 3	56.83
1.588	1	-1 -8 3	58.04
1.584	1	4 -5 2	58.22

Beryllium Calcium Iron Magnesium Aluminum Phosphate Hydroxide Hydrate, Roscherite, $Be_2Ca(Fe_{0.3}Mg_{0.7})_2Al_{0.67}(PO_4)_3(OH)_3 \cdot 2H_2O$

Structure
Monoclinic, C2/c (15), Z = 4. The structure was refined by Fanfani et al. [1975] using material from the U.S. National Museum of Natural History (NMNH #R17847) from Lavra da Ilha, Taquaral (Minas Gerais), Brazil.

Atom positions
Fanfani et al. [1975]

4(a)	2.68 aluminum with 1.32 positions void
4(e)	4 calcium
8(f)	5.6 magnesium plus 2.4 iron
8(f)	8 beryllium
8(f)	8 phosphorus
4(e)	4 phosphorus
8(f)	8 oxygen in each of 6 different sites
8(f)	8 hydroxyl
4(e)	4 hydroxyl
8(f)	8 water

Polymorphism
A triclinic roscherite exists and has a very similar atomic arrangement. Its chemical composition is somewhat different including the replacement of most of the magnesium by manganese [Fanfani et al., 1977].

Lattice constants
a = 15.875(4) Å
b = 11.855(3)
c = 6.605(1)
β = 95.35(3)°

a/b = 1.3391
c/b = 0.5571

(published values: a = 15.874(4) Å, b = 11.854(3), c = 6.605(1), β = 95°21'(2') [Fanfani et al., 1975]).

Volume
1237.6 $Å^3$

Density
(calculated) 2.768 g/cm^3
(measured) 2.766(7) [Fanfani et al., 1975]

Thermal parameters
Isotropic [Fanfani et al., 1975]

Scattering factors
Zero ionization [International Tables, 1962].

Scale factors (integrated intensities)
$\gamma = 0.1851 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 0.654 for reflection with hkℓ = 110.

Additional patterns
1. PDF card 11-355 [Lindberg, 1958]. The data may represent a mixture of the monoclinic and triclinic forms.

References
Fanfani, L., Nunzi, A., Zanazzi, P. F., and Zanzari, A. R. (1975). Tschermak's Mineral. Petrogr. Mitt. 22, 266.
Fanfani, L., Zanazzi, P. F., and Zanzari, A. R. (1977). Tschermak's Mineral. Petrogr. Mitt. 24, 169.
International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.
Lindberg, M. L. (1958). Amer. Mineral. 43, 824.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
9.48	100	1 1 0	9.32
7.89	3	2 0 0	11.20
5.925	83	0 2 0	14.94
5.549	2	-1 1 1	15.96
4.813	31	3 1 0	18.42
4.741	7	2 2 0	18.70
4.401	12	0 2 1	20.16
3.948	3	4 0 0+	22.50
3.831	1	1 3 0	23.20
3.736	4	3 1 1	23.80
3.343	29	-1 3 1	26.64
3.285	15	4 2 0+	27.12
3.160	51	3 3 0	28.22
3.142	46	-2 0 2	28.38
3.054	48	1 1 2+	29.22
2.940	37	2 0 2	30.38
2.915	6	-3 3 1	30.64
2.873	16	0 2 2	31.10
2.854	10	4 2 1	31.32
2.829	16	-3 1 2	31.60
2.774	58	2 4 0	32.24
2.701	3	0 4 1	33.14
2.679	4	5 1 1	33.42
2.633	41	6 0 0	34.02
2.587	3	-2 4 1	34.64
2.527	4	2 4 1+	35.50
2.468	3	1 3 2+	36.38
2.420	6	-4 2 2+	37.12
2.408	12	6 2 0	37.32
2.371	6	4 4 0	37.92
2.345	9	1 5 0+	38.36
2.326	1	-6 2 1	38.68
2.271	6	-4 4 1	39.66
2.258	2	5 3 1	39.90
2.239	2	4 2 2	40.24
2.218	25	7 1 0+	40.64
2.202	13	0 4 2	40.96
2.162	17	-1 1 3+	41.74
2.157	12	-6 0 2+	41.84
2.087	2	2 4 2	43.32

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.062	2	-3 1 3	43.88
2.056	3	0 2 3	44.00
2.046	8	7 1 1	44.24
2.033	8	-2 2 3+	44.52
2.027	10	-6 2 2	44.68
1.976	14	-4 4 2+	45.88
1.971	10	6 4 0	46.00
1.922	8	-1 5 2+	47.26
1.917	8	2 6 0	47.38
1.909	5	5 3 2	47.60
1.892	2	-4 2 3+	48.04
1.885	3	1 3 3	48.24
1.874	2	4 4 2+	48.54
1.868	4	6 2 2	48.70
1.863	3	-5 1 3	48.84
1.846	1	-8 2 1	49.32
1.839	2	7 3 1+	49.54
1.796	2	5 5 1	50.80
1.776	5	3 5 2	51.42
1.767	11	-8 0 2+	51.68
1.763	8	0 4 3+	51.80
1.748	3	-2 4 3	52.30
1.743	7	-6 4 2	52.44
1.739	4	9 1 0	52.58
1.710	2	5 1 3	53.56
1.694	9	0 6 2+	54.10
1.684	2	1 7 0+	54.44
1.673	1	-2 6 2	54.84
1.657	4	-4 4 3	55.42
1.644	21	8 4 0+	55.88
1.640	18	6 4 2+	56.04
1.635	12	-1 7 1+	56.20
1.628	5	1 7 1+	56.48
1.624	3	-8 4 1	56.62
1.612	2	-1 5 3+	57.08
1.605	6	9 3 0+	57.38
1.5904	3	1 5 3+	57.94
1.5804	5	6 6 0+	58.34
1.5765	3	-3 7 1	58.50
1.5696	3	8 2 2	58.78
1.5662	5	8 4 1+	58.92
1.5629	3	7 5 1	59.06
1.5561	2	6 2 3+	59.34
1.5236	1	-7 3 3	60.74
1.5173	4	3 1 4+	61.02
1.5052	2	-7 5 2+	61.56
1.4930	6	-9 3 2+	62.12
1.4802	1	9 1 2+	62.72
1.4676	2	0 6 3	63.32
1.4643	3	-3 7 2	63.48
1.4601	2	-2 6 3	63.68
1.4569	4	-6 6 2+	63.84
1.4420	1	5 7 1	64.58
1.4352	6	-2 4 4+	64.92

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
9.48	100	1 1 0	9.32
7.90	3	2 0 0	11.19
5.927	87	0 2 0	14.93
5.552	2	-1 1 1	15.95
4.815	33	3 1 0	18.41
4.742	5	2 2 0	18.70
4.403	13	0 2 1	20.15
3.953	1	-2 2 1	22.48
3.951	3	4 0 0	22.48
3.834	1	1 3 0	23.18
3.736	5	3 1 1	23.80
3.345	33	-1 3 1	26.63
3.288	5	0 0 2	27.10
3.288	9	4 2 0	27.10
3.280	4	1 3 1	27.17
3.162	8	-1 1 2	28.20
3.161	46	3 3 0	28.21
3.141	46	-2 0 2	28.39
3.054	22	5 1 0	29.21
3.054	34	1 1 2	29.22
3.037	3	-4 2 1	29.39
2.964	5	0 4 0	30.13
2.940	44	2 0 2	30.38
2.914	3	-3 3 1	30.66
2.875	16	0 2 2	31.08
2.871	3	-5 1 1	31.13
2.854	9	4 2 1	31.32
2.830	17	-3 1 2	31.59
2.789	1	3 3 1	32.07
2.776	8	-2 2 2	32.22
2.775	63	2 4 0	32.23
2.702	3	0 4 1	33.13
2.680	4	5 1 1	33.41
2.634	49	6 0 0	34.00
2.634	2	2 2 2	34.01
2.614	2	3 1 2	34.28
2.587	2	-2 4 1	34.64
2.527	4	2 4 1	35.49
2.524	1	-1 3 2	35.54
2.469	1	5 3 0	36.37

Beryllium Calcium Iron Magnesium Aluminum Phosphate Hydroxide Hydrate,
Roscherite, $Be_2Ca(Fe_{0.3}Mg_{0.7})_2Al_{0.67}(PO_4)_3(OH)_3 \cdot 2H_2O$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.468	3	1 3 2	36.37
2.421	4	-4 2 2	37.11
2.419	2	4 0 2	37.14
2.407	14	6 2 0	37.32
2.371	7	4 4 0	37.92
2.345	3	-3 3 2	38.35
2.345	7	1 5 0	38.36
2.325	1	-6 2 1	38.69
2.271	7	-4 4 1	39.65
2.258	2	5 3 1	39.90
2.240	1	4 2 2	40.23
2.218	11	-1 5 1	40.64
2.218	16	7 1 0	40.64
2.218	4	3 3 2	40.65
2.201	13	0 4 2	40.96
2.199	1	1 5 1	41.01
2.192	2	4 4 1	41.15
2.162	18	-1 1 3	41.74
2.162	2	3 5 0	41.74
2.156	1	-6 0 2	41.86
2.156	1	-2 4 2	41.87
2.144	1	5 1 2	42.12
2.087	2	2 4 2	43.31
2.062	1	-3 1 3	43.86
2.056	2	0 2 3	44.01
2.047	1	-5 3 2	44.21
2.046	8	7 1 1	44.24
2.034	7	-2 2 3	44.52
2.031	2	3 5 1	44.58
2.026	8	-6 2 2	44.68
1.976	13	-4 4 2	45.88
1.976	4	0 6 0	45.89
1.976	2	8 0 0	45.89
1.969	2	6 4 0	46.06
1.968	1	6 0 2	46.08
1.923	1	-6 4 1	47.22
1.922	4	-1 3 3	47.26
1.922	4	-1 5 2	47.26
1.917	4	2 6 0	47.39
1.909	4	5 3 2	47.61
1.897	1	5 5 0	47.92
1.893	1	-4 2 3	48.03
1.885	3	1 3 3	48.25
1.874	1	4 4 2	48.54
1.868	4	6 2 2	48.71
1.862	1	-5 1 3	48.87
1.846	1	-8 2 1	49.32
1.838	2	7 3 1	49.54
1.796	2	5 5 1	50.80
1.776	6	3 5 2	51.42

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.768	8	-8 0 2	51.66
1.767	5	4 6 0	51.68
1.762	2	0 4 3	51.83
1.762	1	8 2 1	51.85
1.748	3	-2 4 3	52.29
1.744	7	-6 4 2	52.43
1.737	2	9 1 0	52.64
1.709	2	5 1 3	53.57
1.694	5	-8 2 2	54.09
1.694	6	0 6 2	54.11
1.684	2	1 7 0	54.44
1.673	1	-2 6 2	54.85
1.656	5	-4 4 3	55.43
1.644	10	0 0 4	55.88
1.644	16	8 4 0	55.88
1.643	2	9 1 1	55.93
1.640	1	-2 0 4	56.01
1.640	2	2 6 2	56.03
1.640	4	6 4 2	56.04
1.636	1	-7 1 3	56.18
1.635	7	-1 7 1	56.21
1.628	2	8 0 2	56.48
1.627	2	1 7 1	56.50
1.625	1	-8 4 1	56.60
1.612	1	-1 5 3	57.07
1.605	2	1 1 4	57.37
1.605	6	9 3 0	57.37
1.605	1	5 5 2	57.38
1.5981	1	-9 1 2	57.63
1.5904	3	1 5 3	57.94
1.5806	3	6 6 0	58.33
1.5806	1	10 0 0	58.33
1.5805	1	2 0 4	58.34
1.5764	1	-3 7 1	58.50
1.5697	3	8 2 2	58.78
1.5665	2	8 4 1	58.91
1.5665	2	4 4 3	58.91
1.5623	1	7 5 1	59.08
1.5561	1	6 2 3	59.34
1.5239	1	-7 3 3	60.73
1.5183	1	-4 2 4	60.97
1.5183	1	-8 4 2	60.98
1.5177	1	6 6 1	61.00
1.5168	3	3 1 4	61.04
1.5107	1	3 5 3	61.31
1.5054	1	-5 1 4	61.55
1.5052	1	-7 5 2	61.56
1.4933	3	-9 3 2	62.11
1.4932	2	-3 3 4	62.11
1.4928	1	5 7 0	62.13

Beryllium Calcium Iron Magnesium Aluminum Phosphate Hydroxide Hydrate, Roscherite, $Be_2Ca(Fe_{0.3}Mg_{0.7})_2Al_{0.67}(PO_4)_3(OH)_3 \cdot 2H_2O$ - (continued)

d(Å)	I	hkℓ			2θ(°) λ - 1.540598Å
1.4923	2	7	1	3	62.15
1.4912	2	-8	2	3	62.20
1.4807	1	9	1	2	62.70
1.4676	2	0	6	3	63.32
1.4643	3	-3	7	2	63.48
1.4594	1	-2	6	3	63.72
1.4571	2	-6	0	4	63.83
1.4568	2	-6	6	2	63.85
1.4422	1	5	7	1	64.57
1.4354	1	-10	2	2	64.91
1.4352	7	-2	4	4	64.92

Beryllium Calcium Manganese Aluminum Iron Phosphate Hydroxide Hydrate, Roscherite, $Be_4Ca_2(Mn_{3.91}Mg_{.04}Ca_{.05})(Al_{.13}Fe_{.42}Mn_{.12})(PO_4)_6(OH)_4 \cdot 6H_2O$

Structure
Triclinic, $C\bar{1}$ (2), Z = 2. The structure was refined by Fanfani et al. [1977]. The material used in the structure determination was from Foote Mine, NC.

Atom positions
The trivalent cations Fe, Mn and Al filled only 2/3 of the special positions at 0, 0, ½, the rest being void. All other atoms were in the 4 general positions of the C-centered arrangement [ibid.]. The z coordinate for O(4B) was taken as + 0.1754 and the z coordinate for O(5A) was taken as + 0.9195.

Polymorphism
A monoclinic roscherite exists and has a very similar atomic arrangement with partial disorder of the trivalent cations over the sites (0, 0, 0) and (0, 0, ½). Its chemical composition is somewhat different, including the replacement of most of the manganese by magnesium [Fanfani et al., 1977].

Lattice constants
a = 15.922(5) Å
b = 11.966(4)
c = 6.741(1)
α = 91.07(8)°
β = 94.35(8)
γ = 89.99(8)

(published values: a = 15.921(5) Å, b = 11.965(4), c = 6.741(1), α = 91°4(5)', β = 94°21(5)', γ = 89°59.5(5.0)' [Fanfani et al., 1977]).

CD cell: a = 9.959 Å, b = 9.957, c = 6.741, α = 92.83°, β = 94.12, γ = 73.85, sp. gp. $P\bar{1}$; a/b = 1.0002, c/b = 0.6770

Volume
1280.4 Å^3

Density
(calculated) 2.888 g/cm^3

Thermal parameters
Isotropic [Fanfani et al., 1977]

Scattering factors
Zero ionization [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.1244 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 0.728 for reflection with hkℓ = 020.

References

Fanfani, L., Zanazzi, P. F., and Zanzari, A. R. (1977). Tschermak's Mineral. Petrogr. Mitt. 24, 169.

International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
9.54	100	-1 1 0+	9.26
7.94	11	2 0 0	11.14
6.71	2	0 0 1	13.18
5.981	90	0 2 0	14.80
5.654	11	-1 -1 1	15.66
5.576	4	-1 1 1	15.88
5.342	6	1 1 1+	16.58
4.935	2	2 0 1	17.96
4.839	40	3 1 0+	18.32
4.507	3	0 -2 1	19.68
4.423	10	0 2 1	20.06
4.008	5	-2 -2 1	22.16
3.952	2	-2 2 1	22.48
3.786	5	3 1 1+	23.48
3.404	8	-1 -3 1	26.16
3.353	21	-1 3 1+	26.56
3.307	6	4 2 0+	26.94
3.229	8	-1 -1 2	27.60
3.182	94	-2 0 2+	28.02
3.140	20	1 -1 2	28.40
3.110	18	1 1 2	28.68
3.068	18	-5 1 0+	29.08
3.014	36	2 0 2	29.62
2.992	11	0 4 0	29.84
2.951	5	0 -2 2+	30.26
2.906	5	0 2 2	30.74
2.864	9	-3 -1 2	31.20
2.843	11	-3 1 2	31.44
2.831	9	-2 -2 2	31.58
2.798	48	2 4 0+	31.96
2.751	3	0 -4 1	32.52
2.722	6	5 -1 1	32.88
2.714	6	5 1 1+	32.98
2.682	3	3 -1 2	33.38
2.645	43	6 0 0	33.86
2.593	3	-2 4 1	34.56
2.585	3	-1 -3 2	34.68
2.576	5	2 -4 1	34.80
2.536	6	1 -3 2+	35.36
2.485	4	1 3 2+	36.12
2.474	4	4 0 2	36.28
2.448	2	-4 -2 2	36.68
2.420	14	-6 2 0+	37.12
2.384	9	-3 -3 2+	37.70
2.366	6	-1 5 0+	38.00
2.348	4	-3 3 2	38.30
2.295	2	5 -3 1+	39.22
2.274	4	-4 4 1+	39.60
2.253	11	0 -4 2+	39.98
2.228	22	-1 5 1+	40.46

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.211	20	-1 -1 3+	40.78
2.196	10	-1 1 3+	41.06
2.180	4	3 5 0+	41.38
2.160	4	-6 0 2+	41.78
2.154	3	1 1 3	41.90
2.142	2	2 -4 2	42.16
2.105	2	2 4 2+	42.94
2.095	2	-3 -1 3	43.14
2.076	7	-2 -2 3	43.56
2.072	9	7 -1 1	43.66
2.067	11	7 1 1+	43.76
2.053	4	-2 2 3	44.08
2.046	4	3 5 1+	44.24
2.040	3	-6 -2 2	44.38
2.025	2	-6 2 2	44.72
2.004	6	-4 -4 2+	45.20
1.994	5	0 6 0	45.44
1.984	3	8 0 0	45.68
1.976	4	-4 4 2+	45.88
1.962	2	-1 -5 2	46.24
1.955	3	5 -3 2	46.42
1.933	8	5 3 2+	46.96
1.929	7	-1 5 2+	47.08
1.909	2	6 -2 2+	47.60
1.903	2	-4 2 3	47.76
1.898	2	6 2 2	47.90
1.883	1	8 2 0+	48.30
1.871	1	-5 1 3	48.62
1.867	2	-5 -5 1+	48.74
1.851	1	-8 -2 1+	49.18
1.824	2	5 -5 1	49.96
1.818	2	3 -5 2	50.14
1.808	3	5 5 1+	50.42
1.789	4	3 5 2+	51.02
1.782	6	-4 6 0+	51.22
1.778	5	0 4 3+	51.36
1.769	7	-8 0 2	51.64
1.760	5	-6 -4 2	51.90
1.757	5	-2 4 3	52.02
1.753	5	5 -1 3	52.12
1.742	7	-6 4 2+	52.50
1.729	4	0 -6 2	52.92
1.700	7	0 6 2+	53.88
1.692	3	-8 2 2	54.16
1.685	5	-4 -4 3	54.40
1.680	10	0 0 4	54.58
1.676	8	6 -4 2	54.72
1.654	15	-8 4 0+	55.52
1.640	4	1 1 4+	56.04
1.638	4	1 7 1	56.12
1.633	4	1 -5 3+	56.30
1.627	3	-8 4 1+	56.52
1.622	2	-1 5 3	56.70

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
9.56	57	-1 1 0	9.24
9.55	49	1 1 0	9.25
7.94	11	2 0 0	11.14
6.72	2	0 0 1	13.16
5.982	100	0 2 0	14.80
5.659	12	-1 -1 1	15.65
5.579	3	-1 1 1	15.87
5.346	5	1 1 1	16.57
5.332	1	-2 0 1	16.61
4.947	1	2 0 1	17.91
4.842	21	-3 1 0	18.31
4.837	25	3 1 0	18.33
4.780	1	-2 2 0	18.55
4.774	1	2 2 0	18.57
4.510	3	0 -2 1	19.67
4.427	12	0 2 1	20.04
4.049	1	-3 1 1	21.93
4.009	5	-2 -2 1	22.16
3.953	1	-2 2 1	22.47
3.818	1	3 -1 1	23.28
3.790	4	3 1 1	23.45
3.785	2	2 2 1	23.48
3.406	8	-1 -3 1	26.14
3.360	12	0 0 2	26.50
3.353	13	-1 3 1	26.56
3.353	2	1 -3 1	26.57
3.309	3	-4 2 0	26.92
3.305	3	4 2 0	26.95
3.232	7	-1 -1 2	27.58
3.201	6	-1 1 2	27.85
3.187	33	-3 3 0	27.98
3.183	36	3 3 0	28.01
3.182	51	-2 0 2	28.02
3.140	20	1 -1 2	28.40
3.111	18	1 1 2	28.67
3.070	12	-5 1 0	29.06
3.068	9	5 1 0	29.08
3.013	44	2 0 2	29.62
2.991	8	0 4 0	29.85
2.953	4	0 -2 2	30.24
2.947	2	-3 -3 1	30.31
2.907	5	0 2 2	30.74
2.883	2	4 2 1	30.99
2.877	1	-5 -1 1	31.06
2.865	9	-3 -1 2	31.19

Beryllium Calcium Manganese Aluminum Iron Phosphate Hydroxide Hydrate, Roshcherite, $Be_4Ca_2(Mn_{3.91}Mg_{.04}Ca_{.05})(Al_{.13}Fe_{.42}Mn_{.12})(PO_4)_6(OH)_4 \cdot 6H_2O$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.844	12	-3 1 2	31.43
2.830	6	-2 -2 2	31.59
2.812	1	3 3 1	31.80
2.800	30	-2 4 0	31.94
2.798	31	2 4 0	31.96
2.790	3	-2 2 2	32.06
2.752	2	0 -4 1	32.51
2.723	6	5 -1 1	32.87
2.712	3	5 1 1	33.00
2.710	2	2 -2 2	33.03
2.684	2	3 -1 2	33.36
2.666	1	-4 0 2	33.59
2.665	4	3 1 2	33.60
2.646	55	6 0 0	33.85
2.624	1	-2 -4 1	34.14
2.593	3	-2 4 1	34.56
2.584	1	-1 -3 2	34.69
2.576	4	2 -4 1	34.80
2.543	2	2 4 1	35.26
2.537	2	-1 3 2	35.35
2.537	4	1 -3 2	35.36
2.492	3	1 3 2	36.02
2.486	2	-5 3 0	36.11
2.483	1	5 3 0	36.15
2.474	3	4 0 2	36.29
2.448	3	-4 -2 2	36.68
2.423	2	-4 2 2	37.08
2.421	9	-6 2 0	37.11
2.419	8	6 2 0	37.14
2.390	4	-4 4 0	37.60
2.387	4	4 4 0	37.65
2.384	5	-3 -3 2	37.70
2.366	4	-1 5 0	37.99
2.366	3	1 5 0	38.01
2.349	4	-3 3 2	38.29
2.298	1	4 -2 2	39.17
2.296	1	5 -3 1	39.21
2.294	1	-4 -4 1	39.24
2.274	3	-4 4 1	39.60
2.255	8	0 -4 2	39.95
2.253	7	-1 -5 1	39.99
2.230	1	4 -4 1	40.41
2.229	9	-7 1 0	40.44
2.228	8	7 1 0	40.46
2.227	12	-1 5 1	40.47
2.214	10	0 4 2	40.73
2.211	16	-1 -1 3	40.78
2.208	3	4 4 1	40.84
2.200	1	-2 0 3	40.99
2.198	2	-2 -4 2	41.02
2.196	8	-1 1 3	41.07
2.181	2	-3 5 0	41.36
2.179	2	3 5 0	41.40
2.161	1	-2 4 2	41.77
2.160	4	-6 0 2	41.79
2.152	2	1 1 3	41.95
2.141	2	2 -4 2	42.17
2.105	1	2 4 2	42.94
2.095	1	-3 -1 3	43.14
2.085	2	0 2 3	43.36
2.077	6	-2 -2 3	43.54
2.072	5	7 -1 1	43.65
2.068	2	-5 -3 2	43.74
2.067	8	7 1 1	43.76
2.053	4	-2 2 3	44.08
2.045	2	-5 3 2	44.24
2.044	2	3 5 1	44.27
2.039	2	-6 -2 2	44.40
2.025	2	-6 2 2	44.73
2.006	3	6 0 2	45.16
2.004	5	-4 -4 2	45.20
1.994	6	0 6 0	45.45
1.985	2	8 0 0	45.68
1.977	4	-4 4 2	45.87
1.970	1	-1 -3 3	46.04
1.962	2	-1 -5 2	46.23
1.954	3	5 -3 2	46.43
1.939	2	-1 3 3	46.82
1.938	2	1 -3 3	46.83
1.934	2	-2 6 0	46.93
1.933	3	2 6 0	46.96
1.932	4	5 3 2	46.99
1.928	2	-1 5 2	47.09
1.927	1	-7 -1 2	47.12
1.925	1	-6 4 1	47.17
1.921	1	-4 -2 3	47.28
1.909	1	6 -2 2	47.59
1.902	2	-4 2 3	47.77
1.895	1	6 2 2	47.96
1.872	1	-5 1 3	48.60
1.867	1	-5 -5 1	48.73
1.864	1	7 -3 1	48.81
1.851	1	-8 -2 1	49.19
1.824	2	5 -5 1	49.95
1.818	2	3 -5 2	50.14
1.811	2	4 -2 3	50.34
1.808	3	5 5 1	50.42
1.789	3	3 5 2	51.00
1.788	2	-2 -4 3	51.05
1.783	3	-4 6 0	51.20

Beryllium Calcium Manganese Aluminum Iron Phosphate Hydroxide Hydrate, Roshcherite, $Be_4Ca_2(Mn_{3.91}Mg_{.04}Ca_{.05})(Al_{.13}Fe_{.42}Mn_{.12})(PO_4)_6(OH)_4 \cdot 6H_2O$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.782	1	3 3 3	51.23
1.781	3	4 6 0	51.26
1.777	1	8 2 1	51.36
1.777	2	0 4 3	51.37
1.769	9	-8 0 2	51.64
1.760	5	-6 -4 2	51.90
1.757	3	-2 4 3	52.00
1.753	3	5 -1 3	52.12
1.745	1	-9 1 0	52.38
1.745	1	5 1 3	52.38
1.745	1	9 1 0	52.40
1.742	5	-6 4 2	52.49
1.741	2	2 -4 3	52.51
1.729	6	0 -6 2	52.91
1.705	1	-5 -5 2	53.71
1.701	4	0 6 2	53.86
1.700	3	-8 -2 2	53.89
1.700	1	-1 7 0	53.90
1.699	1	1 7 0	53.92
1.692	2	-8 2 2	54.17
1.685	4	-4 -4 3	54.40
1.680	12	0 0 4	54.58
1.676	3	6 -4 2	54.74
1.670	1	-2 0 4	54.95
1.660	2	-4 4 3	55.29
1.658	4	-1 -7 1	55.37
1.658	1	9 1 1	55.38
1.657	3	6 4 2	55.41
1.655	2	8 0 2	55.49
1.655	9	-8 4 0	55.49
1.653	8	8 4 0	55.56
1.645	2	-7 -1 3	55.84
1.644	3	-1 7 1	55.90
1.638	1	1 1 4	56.11
1.637	2	1 7 1	56.14
1.633	3	1 -5 3	56.30
1.627	1	-3 7 0	56.52
1.627	2	-8 4 1	56.53
1.621	1	-1 5 3	56.74

Calcium Borate Hydrate, Hexahydroborite, $Ca[B(OH)_4]_2 \cdot 2H_2O$

Structure
Monoclinic, P2/a (13), Z = 2. The structure was determined by Simonov et al. [1976], for material from the Solongo deposits in the Urals.

Atom positions
Calcium atoms were in special positions (3/4, 0, z). All other atoms were in general positions [ibid.].

Lattice constants
Simonov et al. [1976]

$a = 8.006(2)$ Å
$b = 8.012(2)$
$c = 6.649(2)$
$\gamma = 104.21(2)°$

CD cell: $a = 8.012$ Å, $b = 6.649$, $c = 8.006$, $\beta = 104.21°$ sp. gp. P2/c; $a/b = 1.2050$, $c/b = 1.2041$

Volume
413.4 Å^3

Density
(calculated) 1.878 g/cm^3

Thermal parameters
Isotropic [Simonov et al., 1976]

Scattering factors
B^0, Ca^0, O^- [Cromer and Mann, 1968].
H^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.4656 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 1.05 for reflection with hkℓ = 010.

Additional pattern
1. PDF card 23-866 [Gode and Kuka, 1970]

References

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International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.
Simonov, M. A., Yamanova, N. A., Kazanskaya, E. V., Egorov - Tismenko, Yu. K., and Belov, N. V. (1976). Sov. Phys. Dokl. 21, 314.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
7.76	100	0 1 0	11.40
6.64	38	0 0 1	13.32
5.046	12	0 1 1	17.56
4.576	13	-1 1 1	19.38
3.952	20	1 1 1	22.48
3.877	6	0 2 0+	22.92
3.346	76	-1 2 1+	26.62
3.173	14	2 1 0	28.10
3.056	4	0 1 2	29.20
2.855	7	-2 2 1+	31.30
2.754	1	1 1 2	32.48
2.589	2	0 3 0	34.62
2.524	43	2 0 2	35.54
2.468	35	-3 1 1+	36.38
2.413	13	0 3 1	37.24
2.295	23	2 1 2+	39.22
2.216	2	0 0 3	40.68
2.167	7	1 3 1	41.64
2.131	3	0 1 3+	42.38
2.092	1	-1 1 3	43.22
2.076	4	-3 1 2	43.56
2.042	1	0 3 2+	44.32
2.021	2	1 1 3	44.82
1.971	16	-2 3 2	46.00
1.941	10	0 4 0	46.76
1.936	12	-4 2 0+	46.88
1.924	11	-2 1 3+	47.20
1.863	10	4 0 1+	48.86
1.817	8	1 2 3+	50.16
1.782	3	4 1 0	51.22
1.776	8	-4 3 0	51.42
1.722	3	4 1 1	53.16
1.716	3	-4 3 1	53.34
1.703	2	-1 3 3	53.80
1.683	1	3 0 3+	54.48
1.678	3	3 2 2+	54.66
1.674	4	-2 4 2+	54.80
1.662	3	0 0 4	55.22
1.646	3	2 2 3	55.80
1.625	2	0 1 4+	56.58
1.608	1	-1 1 4	57.26
1.587	3	4 2 0	58.08
1.571	1	4 1 2+	58.72
1.553	4	0 5 0+	59.46
1.544	2	2 4 1	59.86
1.537	2	-4 4 1	60.14
1.528	2	2 0 4+	60.56
1.4853	1	-4 1 3	62.48
1.4709	1	1 2 4+	63.16
1.4676	1	-3 5 1	63.32

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.4618	2	2 3 3+	63.60
1.4325	1	2 4 2	65.06
1.4286	2	-2 5 2+	65.26
1.4094	1	-1 3 4	66.26

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
7.77	100	0 1 0	11.38
6.65	38	0 0 1	13.31
5.051	13	0 1 1	17.54
4.581	14	-1 1 1	19.36
3.955	21	1 1 1	22.46
3.883	3	0 2 0	22.88
3.881	2	2 0 0	22.90
3.872	3	-2 1 0	22.95
3.353	27	0 2 1	26.56
3.351	16	2 0 1	26.58
3.347	27	-1 2 1	26.61
3.346	24	-2 1 1	26.62
3.324	7	0 0 2	26.79
3.174	16	2 1 0	28.09
3.056	4	0 1 2	29.20
2.865	3	1 2 1	31.19
2.864	2	2 1 1	31.20
2.854	6	-2 2 1	31.32
2.754	2	1 1 2	32.48
2.589	3	0 3 0	34.62
2.525	46	2 0 2	35.53
2.523	6	-1 2 2	35.55
2.469	19	-1 3 1	36.35
2.468	25	-3 1 1	36.37
2.460	1	2 2 0	36.50
2.449	2	-2 3 0	36.67
2.413	15	0 3 1	37.24
2.411	2	3 0 1	37.27
2.298	2	-2 3 1	39.17
2.297	2	-3 2 1	39.18
2.296	3	1 2 2	39.20
2.296	22	2 1 2	39.21
2.290	3	-2 2 2	39.30
2.216	2	0 0 3	40.68
2.168	8	1 3 1	41.63
2.131	3	0 1 3	42.38
2.131	1	1 0 3	42.38
2.091	1	-1 1 3	43.22
2.076	5	-3 1 2	43.56
2.043	1	0 3 2	44.31
2.021	3	1 1 3	44.82
1.977	8	2 2 2	45.86
1.972	16	-2 3 2	45.99
1.971	1	-3 2 2	46.00
1.942	10	0 4 0	46.75
1.937	3	-2 4 0	46.86
1.936	6	-4 2 0	46.89
1.925	3	0 2 3	47.18
1.925	2	2 0 3	47.19
1.924	2	-1 2 3	47.21
1.924	6	-2 1 3	47.21
1.917	1	-4 1 1	47.40
1.866	4	2 3 1	48.75
1.866	3	3 2 1	48.76
1.864	2	0 4 1	48.82
1.863	6	4 0 1	48.86
1.860	1	-2 4 1	48.94
1.817	9	1 2 3	50.16
1.815	5	-2 2 3	50.24
1.782	2	4 1 0	51.21
1.776	10	-4 3 0	51.41
1.722	3	4 1 1	53.16
1.716	2	-4 3 1	53.35
1.703	3	-1 3 3	53.80
1.683	1	3 0 3	54.47
1.678	2	3 2 2	54.65
1.674	4	-2 4 2	54.80
1.662	4	0 0 4	55.21
1.646	4	2 2 3	55.79
1.625	2	0 1 4	56.58
1.608	1	-1 1 4	57.26
1.587	4	4 2 0	58.08
1.571	1	4 1 2	58.73
1.555	2	-5 1 1	59.39
1.553	4	0 5 0	59.46
1.544	3	2 4 1	59.85
1.537	1	-4 4 1	60.14
1.4854	1	-4 1 3	62.47
1.4726	1	1 2 4	63.08
1.4676	1	-3 5 1	63.32
1.4617	2	2 3 3	63.60
1.4326	1	2 4 2	65.06
1.4288	1	-2 5 2	65.25
1.4271	1	-4 4 2	65.34
1.4096	1	-1 3 4	66.25

Calcium Chromium Iron Titanium Oxide, Loveringite, $Ca_{.72}RE_{.33}(Y,Th,U,Pb)_{.05}Ti_{12.48}Fe_{3.38}Cr_{2.24}Mg_{.92}Zr_{.58}Al_{.39}V_{.21}Mn_{.04}O_{38}$

Structure
Hexagonal, $R\bar{3}$ (148), Z = 3, isostructural with senaite. The structure was refined by Gatehouse et al. [1978] using rhombohedral positions. Those were used to calculate the powder pattern which was transformed to the hexagonal setting given here. The sample used for the structure work came from the Jimberlana Intrusion near Norseman, Western Australia.

Atom positions
M(0) in 1(a) .72 calcium +.23 RE (as .1284 lanthanum and .1016 cerium) +.017 lead +.014 yttrium +.011 uranium +.006 thorium
M(1) in 1(b) .58 zirconium +.32 magnesium +.1 RE (as .0285 hafnium, .0259 cerium, .0245 neodymium and .0236 holmium)
M(2) in 2(c) partially vacant, with 1.23 iron and 0.6 magnesium
M(3) in 6(f) partially vacant, with 2.24 chromium +2.19 iron +.86 titanium +.21 vanadium
M(4) in 6(f) 5.81 titanium and .19 aluminum
M(5) in 6(f) 5.81 titanium and .19 aluminum
6(f) 6 oxygen in each of 6 different sites
2(c) 2 oxygen

Electron microprobe analysis results gave weight percents of the elements as oxides, and the unit cell composition was normalized to 38 oxygen. Distribution of the cations in sites M(0) to M(5) inclusive was guided by the results for senaite and crichtonite which showed ordering sequences based on the size of the cations [Gatehouse et al., 1978]. The Mn was combined with the Fe in sites M(2) and M(3).

Lattice constants
a = 10.337 Å
c = 20.676

c/a = 2.0002

(published values: a = 9.117(4) Å, α = 69.07(1)° [Gatehouse et al., 1978])

Volume
1913.4 $Å^3$

Density
(calculated) 4.415 g/cm^3

Thermal parameters
Isotropic [Gatehouse et al., 1978]

Scattering factors
Al^{3+}, Ce^{4+}, Cr^{3+}, Fe^{3+}, Hf^{4+}, Ho^{3+}, La^{3+}, Mg^{2+}, Nd^{3+}, O^{1-}, Pb^{2+}, Th^{4+}, Ti^{4+}, U^{4+}, V^{5+}, Y^{3+}, Zr^{4+} [International Tables, 1974]
Ca^{2+} [Cromer and Mann, 1968]
The factors for cerium, lanthanum and zirconium were corrected for dispersion [Cromer and Liberman, 1970]

Scale factors (integrated intensities)
$\gamma = 0.06676 \times 10^{-3}$
$I/I_{corundum} = 0.624$, for reflection with hexagonal hkℓ = 024.

References
Cromer, D. R. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.
Gatehouse, B. M., Grey, I. E., Campbell, I. H., and Kelly, P. (1978). Amer. Mineral. 63, 28.
International Tables for X-ray Crystallography, IV (1974). (The Kynoch Press, Birmingham, Eng.) p. 99.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
6.89	1	0 0 3	12.84
5.16	1	1 1 0	17.16
4.476	9	1 0 4	19.82
4.371	3	0 2 1	20.30
4.134	23	1 1 -3+	21.48
3.751	13	0 1 5	23.70
3.443	3	0 0 6	25.86
3.383	75	0 2 4	26.32
3.339	7	2 1 1	26.68
3.216	5	1 2 2	27.72
3.038	71	2 0 5	29.38
2.984	31	3 0 0	29.92
2.866	100	1 1 -6+	31.18
2.831	72	1 2 -4+	31.58
2.807	12	1 0 7	31.86
2.738	31	0 3 3+	32.68
2.618	40	1 2 5+	34.22
2.585	9	2 2 0	34.68
2.465	53	3 1 -1	36.42
2.414	28	3 1 2+	37.22
2.297	2	0 0 9	39.18
2.238	57	3 1 -4+	40.26
2.128	59	3 1 5+	42.44
2.099	5	1 1 -9+	43.06
2.054	3	1 2 8+	44.06
2.015	4	1 0 10+	44.96
1.968	1	0 4 5	46.08
1.954	7	1 4 0+	46.44
1.909	12	2 3 -4	47.60
1.901	16	3 1 -7	47.82
1.878	6	0 2 10+	48.42
1.839	17	2 3 5	49.52
1.791	50	3 1 8	50.96
1.764	10	2 1 10	51.78
1.723	4	0 0 12	53.12

Calcium Chromium Iron Titanium Oxide, Loveringite,
$Ca_{.72}RE_{.33}(Y,Th,U,Pb)_{.05}Ti_{12.48}Fe_{3.38}Cr_{2.24}Mg_{.92}Zr_{.58}Al_{.39}V_{.21}Mn_{.04}O_{38}$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.700	25	1 4 6+	53.90
1.686	8	2 4 1+	54.36
1.643	11	5 0 5	55.92
1.635	4	1 1 -12+	56.22
1.608	10	4 2 -4+	57.26
1.589	61	3 1 -10	58.00
1.566	9	4 2 5+	58.94
1.541	10	3 3 -6+	59.98
1.535	9	5 1 4+	60.22
1.519	2	4 0 10	60.96
1.4987	28	3 1 11+	61.86
1.4883	3	4 1 9+	62.34
1.4717	1	5 0 8	63.12
1.4680	2	2 4 7+	63.30
1.4573	6	6 0 3+	63.82
1.4392	8	2 1 13+	64.72
1.4336	61	2 5 0	65.00
1.4155	6	4 3 4	65.94
1.4030	7	2 0 14+	66.60
1.3865	6	4 3 -5+	67.50
1.3782	2	3 3 -9+	67.96
1.3690	10	0 6 6+	68.48
1.3535	5	1 2 14+	69.38
1.3393	6	3 1 -13+	70.22
1.3317	5	1 1 -15	70.68
1.3236	2	5 2 -6+	71.18
1.3200	2	6 1 -4	71.40
1.3172	2	3 4 -7+	71.58
1.3093	2	2 4 10	72.08
1.2962	2	6 1 5+	72.92
1.2923	3	1 4 12+	73.18
1.2694	2	1 3 -14+	74.72
1.2574	1	2 4 -11+	75.56
1.2515	1	3 0 15+	75.98
1.2415	3	0 2 16+	76.70
1.2390	6	6 2 1	76.88
1.2325	2	6 2 -2	77.36
1.2216	3	0 7 5+	78.18
1.2185	3	3 3 -12+	78.42
1.2162	5	2 5 -9+	78.60
1.2097	3	4 4 6+	79.10
1.2072	6	1 2 -16+	79.30
1.1991	4	2 3 14+	79.94
1.1890	2	6 2 -5	80.76
1.1861	2	7 1 0	81.00

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
6.80	1	0 0 3	12.83
5.17	1	1 1 0	17.14
4.476	11	1 0 4	19.82
4.375	3	0 2 1	20.28
4.135	11	1 1 3	21.47
4.135	16	1 1 -3	21.47
4.108	9	2 0 2	21.62
3.754	16	0 1 5	23.68
3.446	2	0 0 6	25.83
3.384	100	0 2 4	26.32
3.339	6	2 1 1	26.67
3.216	6	1 2 2	27.72
3.037	97	2 0 5	29.38
2.984	40	3 0 0	29.92
2.867	56	1 1 6	31.17
2.867	80	1 1 -6	31.17
2.831	16	2 1 4	31.58
2.831	80	1 2 -4	31.58
2.805	8	1 0 7	31.88
2.738	22	3 0 3	32.68
2.738	20	0 3 3	32.68
2.619	47	1 2 5	34.21
2.619	10	2 1 -5	34.21
2.584	12	2 2 0	34.68
2.465	1	0 2 7	36.41
2.465	3	1 3 1	36.42
2.465	72	3 1 -1	36.42
2.420	12	2 2 3	37.12
2.420	11	2 2 -3	37.12
2.414	23	3 1 2	37.21
2.297	3	0 0 9	39.18
2.238	29	1 3 4	40.26
2.238	55	3 1 -4	40.26
2.225	2	2 1 7	40.51
2.225	2	1 2 -7	40.51
2.129	73	3 1 5	42.43
2.129	15	1 3 -5	42.43
2.099	3	1 1 9	43.05
2.099	4	1 1 -9	43.05
2.054	3	1 2 8	44.05
2.054	1	2 1 -8	44.05
2.015	3	1 0 10	44.96
2.014	2	2 3 2	44.96
1.968	1	0 4 5	46.08
1.954	8	1 4 0	46.45
1.954	4	4 1 0	46.45
1.909	1	3 2 4	47.61
1.909	16	2 3 -4	47.61
1.901	20	3 1 -7	47.82
1.879	2	1 4 3	48.39

Calcium Chromium Iron Titanium Oxide, Loveringite,
$Ca_{.72}RE_{.33}(Y,Th,U,Pb)_{.05}Ti_{12.48}Fe_{3.38}Cr_{2.24}Mg_{.92}Zr_{.58}Al_{.39}V_{.21}Mn_{.04}O_{38}$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.879	3	4 1 3	48.39
1.879	2	4 1 -3	48.39
1.877	5	0 2 10	48.46
1.840	1	0 1 11	49.51
1.839	25	2 3 5	49.51
1.791	1	1 3 -8	50.96
1.791	76	3 1 8	50.96
1.784	1	4 0 7	51.17
1.784	1	5 0 -1	51.17
1.764	13	2 1 10	51.77
1.723	5	0 0 12	53.11
1.699	3	4 1 6	53.91
1.699	18	1 4 6	53.91
1.699	17	1 4 -6	53.91
1.699	1	4 1 -6	53.91
1.692	7	0 5 4	54.17
1.686	2	2 3 -7	54.36
1.686	1	3 2 7	54.36
1.686	4	2 4 1	54.37
1.643	1	1 2 11	55.91
1.643	17	5 0 5	55.92
1.635	2	1 1 12	56.23
1.635	2	1 1 -12	56.23
1.608	1	3 2 -8	57.25
1.608	5	2 4 4	57.25
1.608	8	4 2 -4	57.25
1.603	1	1 5 -1	57.44
1.589	1	1 3 10	58.00
1.589	95	3 1 -10	58.00
1.589	1	5 1 -2	58.00
1.566	2	1 0 13	58.93
1.566	7	4 2 5	58.94
1.566	5	2 4 -5	58.94
1.541	6	3 3 6	59.98
1.541	9	3 3 -6	59.98
1.535	3	1 5 -4	60.23
1.535	8	5 1 4	60.23
1.519	3	4 0 10	60.96
1.4986	39	3 1 11	61.86
1.4986	2	1 5 5	61.86
1.4986	3	5 1 -5	61.86
1.4920	1	6 0 0	62.17
1.4882	1	4 1 9	62.34
1.4718	1	5 0 8	63.12
1.4680	2	2 4 7	63.30
1.4582	4	6 0 3	63.77
1.4571	2	3 2 10	63.83
1.4571	1	2 3 -10	63.83
1.4570	4	4 3 -2	63.83
1.4394	4	1 2 -13	64.71
1.4394	4	2 1 13	64.71
1.4335	96	2 5 0	65.01
1.4335	5	5 2 0	65.01
1.4155	8	4 3 4	65.94
1.4122	1	1 5 -7	66.11
1.4035	3	5 2 -3	66.58
1.4035	3	5 2 3	66.58
1.4025	6	2 0 14	66.63
1.3865	1	3 4 5	67.50
1.3865	7	4 3 -5	67.50
1.3783	1	3 3 -9	67.95
1.3692	9	6 0 6	68.47
1.3692	7	0 6 6	68.47
1.3536	4	2 1 -14	69.37
1.3536	3	1 2 14	69.37
1.3393	7	1 3 13	70.22
1.3393	2	3 1 -13	70.22
1.3319	7	1 1 15	70.67
1.3319	1	1 1 -15	70.67
1.3235	1	5 2 -6	71.18
1.3199	1	6 1 -4	71.41
1.3173	1	4 3 7	71.57
1.3173	1	3 4 -7	71.57
1.3093	2	2 4 10	72.07
1.2965	1	4 0 13	72.91
1.2964	1	6 1 5	72.91
1.2922	2	1 4 12	73.18
1.2922	2	2 4 -12	73.18
1.2693	1	3 1 14	74.73
1.2693	1	1 3 -14	74.73
1.2693	1	1 5 -10	74.73
1.2514	1	3 0 15	75.99
1.2514	1	0 3 15	75.99
1.2416	2	0 2 16	76.69
1.2414	2	7 0 4	76.70
1.2392	7	6 2 1	76.87
1.2326	2	6 2 -2	77.36
1.2218	5	0 7 5	78.17
1.2162	1	5 2 9	78.60
1.2162	1	2 5 -9	78.60
1.2162	2	2 5 9	78.60
1.2162	2	5 2 -9	78.60
1.2099	2	4 4 6	79.09
1.2099	3	4 4 -6	79.09
1.2072	5	1 2 -16	79.30
1.2071	3	6 2 4	79.31
1.1990	3	2 3 14	79.95
1.1990	1	3 4 -10	79.95
1.1990	1	4 3 10	79.95
1.1890	4	6 2 -5	80.76

Calcium Hydrogen Phosphate Sulfate Hydrate, $Ca_2HPO_4SO_4 \cdot 4H_2O$

Structure
Monoclinic, Cc (9), Z = 4. The structure was determined by Sakae et al. [1978].

Atom positions
4(a) 2 phosphorus(1) and 2 sulfur(1)
4(a) 2 phosphorus(2) and 2 sulfur(2)

Four hydrogen atoms were not located in the structure determination. All other atoms are in general positions 4(a) and the "x" and "z" parameters were given to only 3 significant figures [ibid.].

Lattice constants
a = 5.721(5) Å
b = 30.994(5)
c = 6.250(4)
β = 117.26(6)°

(published values: a = 5.721(5) Å, b = 30.992(5), c = 6.250(4), β = 117.26(6)° [Sakae et al., 1978]).

CD cell: a = 6.248(4) Å, b = 30.994(5), c = 5.721(5), β = 117.22(6)°, sp. gp. Aa(9); a/b = 0.2016, c/b = 0.1846.

Volume
985.15 Å^3

Density
(calculated) 2.321 g/cm^3

Thermal parameters
Isotropic [Sakae et al., 1978]

Scattering factors
Zero ionization [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 0.3683 \times 10^{-3}$

References
International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.
Sakae, T., Nagate, H., and Sudo, T. (1978). Amer. Mineral. 63, 520.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
7.74	100	0 4 0	11.42
5.02	5	-1 1 1+	17.66
4.56	40	1 3 0+	19.44
3.931	50	-1 5 1+	22.60
3.874	15	0 8 0	22.94
3.783	1	0 6 1	23.50
3.339	45	1 7 0+	26.68
3.093	10	-1 1 2+	28.84
2.976	15	-1 3 2+	30.00
2.852	35	-1 9 1+	31.34
2.812	10	-2 2 1	31.80
2.779	15	1 5 1+	32.18
2.733	15	0 2 2	32.74
2.707	1	0 10 1	33.06
2.615	5	0 4 2	34.26
2.543	15	2 0 0+	35.26
2.509	5	2 2 0+	35.76
2.447	20	0 6 2	36.70
2.416	5	-2 4 2+	37.18
2.308	5	-1 9 2+	39.00
2.282	5	2 6 0+	39.46
2.158	1	-1 13 1+	41.82
2.126	5	2 8 0+	42.48
2.102	10	-2 10 1	43.00
2.088	5	-1 11 2+	43.30
2.068	5	0 10 2+	43.74
2.031	5	-1 3 3+	44.58
1.976	5	-2 2 3+	45.88
1.966	10	-2 10 2+	46.14
1.936	1	0 16 0	46.88
1.930	5	2 4 1+	47.04
1.892	5	0 12 2+	48.06
1.876	5	1 7 2+	48.48
1.849	1	-3 3 2+	49.24
1.829	1	0 16 1	49.82
1.812	15	-2 12 2+	50.32
1.798	5	-3 5 1+	50.72
1.775	5	1 9 2+	51.44
1.731	10	0 14 2+	52.86
1.716	5	-1 17 1+	53.34
1.669	5	-1 11 3+	54.96
1.650	1	-3 9 1+	55.66
1.646	1	0 18 1	55.82
1.635	1	-3 5 3+	56.20
1.583	1	-3 7 3+	58.22
1.573	1	-1 17 2+	58.66
1.564	1	-1 13 3+	59.02
1.554	1	-2 0 4+	59.44
1.547	5	-2 2 4+	59.74
1.541	5	-2 16 2+	59.98

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
7.75	100	0 4 0	11.41
5.02	1	-1 1 1	17.65
5.02	1	1 1 0	17.66
4.56	20	-1 3 1	19.43
4.56	20	1 3 0	19.44
4.52	1	0 4 1	19.65
3.932	30	-1 5 1	22.59
3.932	30	1 5 0	22.60
3.874	15	0 8 0	22.94
3.783	1	0 6 1	23.50
3.340	25	-1 7 1	26.67
3.339	25	1 7 0	26.67
3.094	5	-1 1 2	28.83
3.093	5	1 1 1	28.84
2.978	10	-1 3 2	29.98
2.977	10	1 3 1	29.99
2.852	20	-1 9 1	31.34
2.852	20	1 9 0	31.34
2.813	10	-2 2 1	31.79
2.780	10	-1 5 2	32.18
2.779	10	1 5 1	32.19
2.734	15	0 2 2	32.72
2.707	1	0 10 1	33.07
2.615	10	0 4 2	34.26
2.545	5	-1 7 2	35.24
2.544	5	1 7 1	35.25
2.544	5	-2 0 2	35.26
2.543	5	2 0 0	35.27
2.510	5	-2 2 2	35.74
2.509	5	2 2 0	35.76
2.502	1	-2 6 1	35.86
2.447	25	0 6 2	36.70
2.417	1	-2 4 2	37.17
2.416	1	2 4 0	37.18
2.308	5	-1 9 2	38.99
2.308	5	1 9 1	39.00
2.282	1	-2 6 2	39.46
2.281	5	2 6 0	39.47
2.159	1	-1 13 1	41.81
2.159	1	1 13 0	41.81
2.126	5	-2 8 2	42.48
2.126	5	2 8 0	42.49
2.102	10	-2 10 1	42.99
2.088	1	-1 11 2	43.30
2.088	1	1 11 1	43.30
2.069	5	0 10 2	43.72
2.031	5	-1 3 3	44.57
2.031	5	1 3 2	44.58
1.977	1	-2 2 3	45.86
1.976	1	2 2 1	45.88
1.966	5	-2 10 2	46.13
1.966	5	2 10 0	46.14
1.965	1	-1 5 3	46.16
1.964	1	1 5 2	46.17
1.937	1	0 16 0	46.86
1.930	5	-2 4 3	47.04
1.930	5	2 4 1	47.05
1.892	5	0 12 2	48.06
1.877	1	-1 7 3	48.47
1.876	1	-3 1 2	48.48
1.876	5	1 7 2	48.48
1.876	1	-3 1 1	48.49
1.829	1	0 16 1	49.81
1.812	10	-2 12 2	50.31
1.812	10	2 12 0	50.31
1.799	5	-3 5 2	50.71
1.799	5	-3 5 1	50.72
1.775	5	-1 9 3	51.43
1.775	5	1 9 2	51.44
1.731	5	0 14 2	52.84
1.730	1	-3 7 2	52.87
1.730	1	-3 7 1	52.88
1.716	1	-1 17 1	53.34
1.716	1	1 17 0	53.34
1.670	1	-2 14 2	54.94
1.670	1	2 14 0	54.95
1.669	1	-1 11 3	54.97
1.669	1	1 11 2	54.98
1.650	1	-3 9 2	55.66
1.650	1	-3 9 1	55.67
1.645	1	0 18 1	55.85
1.584	1	-3 7 3	58.21
1.573	1	-1 17 2	58.65
1.573	1	1 17 1	58.66
1.547	5	-2 2 4	59.72
1.547	1	2 2 2	59.75
1.541	1	-2 16 2	59.98
1.541	1	2 16 0	59.99

Cannabidiol, $C_{21}H_{30}O_2$

Synonym
1. (1R-trans)-2-[3-Methyl-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl-1,3-benezenediol

CAS registry no.
13956-29-1

Structure
Monoclinic, $P2_1$ (4), Z = 4. The structure was refined by Jones et al. [1977].

Atom positions
All atoms were in general positions 2(a). Sixty-eight hydrogen positions were not located.

Lattice constants
a = 10.618(4) Å
b = 10.650(5)
c = 17.267(6)
β = 95.30(4)°

(published values: a = 10.617(4) Å, b = 10.649(5), c = 17.266(6), β = 95.30(4)° [Jones et al., 1977])

CD cell: a = 17.267(6) Å, b = 10.650(5), c = 10.618(4), β = 95.30(4)°; sp. gp. $P2_1$; a/b = 1.6213; c/b = 0.9970

Volume
1944.2 Å^3

Density
(calculated) 1.074 g/cm^3 [Jones et al., 1977]

Thermal parameters
Isotropic. For hydrogen atoms, overall B = 0.125. For other atoms, B_i were estimated from U_{ij} for individual atoms.

Scattering factors
Zero ionization [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 2.067 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 0.668 for reflections with hkℓ = 011.

References

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Jones, P. G., Falvello, L., Kennard, O., Sheldrick, G. M., and Mechoulam, R. (1977). Acta. Crystallogr. B33, 3211.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
17.18	4	0 0 1	5.14
10.57	5	1 0 0	8.36
9.40	32	-1 0 1	9.40
9.05	100	0 1 1	9.76
8.60	33	0 0 2	10.28
7.494	33	1 1 0	11.80
7.042	19	-1 1 1	12.56
6.702	30	1 1 1+	13.20
6.384	20	1 0 2	13.86
5.840	20	-1 1 2	15.16
5.727	4	0 0 3	15.46
5.474	3	1 1 2	16.18
5.323	5	0 2 0	16.64
5.187	6	-2 0 1	17.08
5.081	34	0 2 1	17.44
4.924	10	2 0 1	18.00
4.701	28	-1 1 3+	18.86
4.662	22	-2 1 1	19.02
4.530	11	1 2 1+	19.58
4.471	5	2 1 1	19.84
4.296	20	-2 1 2+	20.66
4.235	10	-1 2 2	20.96
4.085	23	1 2 2	21.74
4.005	24	2 1 2	22.18
3.987	26	0 1 4	22.28
3.901	15	0 2 3	22.78
3.860	3	1 0 4	23.02
3.841	3	-1 1 4	23.14
3.808	2	-2 1 3	23.34
3.736	7	-1 2 3+	23.80
3.717	8	2 0 3+	23.92
3.628	7	1 1 4	24.52
3.587	4	1 2 3	24.80
3.498	6	-2 0 4+	25.44
3.477	4	0 3 1	25.60
3.388	1	3 0 1	26.28
3.358	3	2 2 2+	26.52
3.341	3	-3 1 1+	26.66
3.321	3	-2 1 4+	26.82
3.283	3	1 3 1	27.14
3.257	2	-1 2 4	27.36
3.232	4	3 1 1+	27.58
3.213	5	-3 1 2+	27.74
3.160	2	3 0 2+	28.22
3.123	2	1 2 4	28.56
3.102	4	1 3 2	28.76
3.052	7	2 1 4+	29.24
3.010	1	-3 1 3+	29.66
2.923	1	-2 2 4+	30.56
2.897	1	-2 1 5	30.84

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.859	3	1 3 3+	31.26
2.735	2	1 2 5+	32.72
2.717	1	3 2 2	32.94
2.677	2	2 1 5+	33.44
2.662	1	0 4 0	33.64
2.621	3	1 1 6+	34.18
2.593	2	-4 0 2	34.56
2.582	3	1 4 0+	34.72
2.562	2	-1 4 1+	35.00
2.535	3	3 1 4+	35.38
2.499	1	-3 3 1+	35.90
2.452	1	3 3 1+	36.62
2.445	1	-3 3 2+	36.72
2.424	1	-4 1 3+	37.06
2.410	1	1 2 6	37.28
2.373	1	-1 4 3+	37.88
2.349	1	-3 3 3+	38.28
2.277	1	-3 1 6	39.54
2.235	1	3 3 3+	40.32
2.219	1	-1 2 7	40.62
2.214	2	-1 3 6	40.72
2.147	1	1 2 7+	42.06
2.119	1	-2 2 7+	42.64
2.088	1	-1 4 5+	43.30
2.004	1	-4 1 6+	45.22
1.997	1	0 5 3+	45.38
1.971	1	-2 5 1+	46.00
1.936	1	-2 3 7+	46.88
1.748	1	5 3 2+	52.28

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
17.19	3	0 0 1	5.14
10.57	5	1 0 0	8.36
9.40	29	-1 0 1	9.40
9.05	100	0 1 1	9.76
8.66	4	1 0 1	10.21
8.60	30	0 0 2	10.28
7.503	34	1 1 0	11.79
7.048	19	-1 1 1	12.55
6.717	21	1 1 1	13.17
6.689	14	0 1 2	13.23
6.387	20	1 0 2	13.85
5.846	20	-1 1 2	15.14
5.731	3	0 0 3	15.45
5.478	3	1 1 2	16.17
5.325	5	0 2 0	16.63
5.189	5	-2 0 1	17.07
5.087	35	0 2 1	17.42
5.047	4	0 1 3	17.56
4.927	10	2 0 1	17.99
4.735	4	2 1 0	18.72
4.706	14	-1 1 3	18.84
4.701	13	-2 0 2	18.86
4.665	18	-2 1 1	19.01
4.633	6	-1 2 1	19.14
4.536	8	1 2 1	19.56
4.527	3	0 2 2	19.59
4.471	5	2 1 1	19.84
4.328	1	2 0 2	20.50
4.301	14	-2 1 2	20.64
4.298	7	0 0 4	20.65
4.237	10	-1 2 2	20.95
4.090	21	1 2 2	21.71
4.078	6	-2 0 3	21.78
4.010	22	2 1 2	22.15
3.986	23	0 1 4	22.29
3.901	16	0 2 3	22.78
3.859	2	1 0 4	23.03
3.840	2	-1 1 4	23.15
3.808	1	-2 1 3	23.34
3.752	3	2 2 0	23.70
3.737	5	-1 2 3	23.79
3.718	5	2 0 3	23.91
3.716	2	-2 2 1	23.92
3.628	7	1 1 4	24.51
3.616	1	2 2 1	24.60
3.587	3	1 2 3	24.80
3.524	2	-2 2 2	25.25
3.511	3	2 1 3	25.35
3.497	4	-2 0 4	25.45
3.477	3	0 3 1	25.60
3.391	1	3 0 1	26.26
3.363	1	-1 0 5	26.49
3.359	2	2 2 2	26.52
3.345	1	0 2 4	26.63
3.340	1	-3 1 1	26.67
3.322	2	-2 1 4	26.81
3.285	2	1 3 1	27.13
3.257	1	-1 2 4	27.36
3.238	2	-2 2 3	27.53
3.231	2	3 1 1	27.58
3.215	4	-3 1 2	27.73
3.207	2	-1 1 5	27.80
3.194	1	2 0 4	27.91
3.160	1	3 0 2	28.22
3.125	2	1 2 4	28.54

Cannabidiol, $C_{21}H_{30}O_2$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
3.103	4	1 3 2	28.75
3.059	6	2 1 4	29.17
3.051	3	1 1 5	29.25
3.049	1	2 2 3	29.27
3.029	1	3 1 2	29.46
2.923	1	-2 2 4	30.56
2.899	1	-2 1 5	30.82
2.865	2	1 3 3	31.19
2.860	2	3 2 1	31.24
2.858	1	-3 0 4	31.27
2.849	1	-3 2 2	31.38
2.733	1	1 2 5	32.74
2.718	1	3 2 2	32.93
2.679	2	2 1 5	33.42
2.662	1	0 4 0	33.63
2.631	1	0 4 1	34.05
2.623	1	-2 0 6	34.16
2.620	1	1 1 6	34.19
2.613	1	1 3 4	34.29
2.595	2	-4 0 2	34.54
2.582	3	1 4 0	34.72
2.562	2	-1 4 1	35.00
2.537	1	3 2 3	35.35
2.535	2	3 1 4	35.38
2.445	1	-3 3 2	36.73
2.424	1	-4 1 3	37.06
2.411	1	1 2 6	37.27
2.374	1	-1 4 3	37.86
2.277	1	-3 1 6	39.54
2.220	1	-1 2 7	40.60
2.214	1	-1 3 6	40.72
2.120	1	-2 2 7	42.62

L-Cocaine Hydrochloride, $C_{17}H_{22}ClNO_4$

Synonyms
1. L-3-Tropanylbenzoate-2-carboxylic acid methyl ester hydrochloride
2. Cocaine muriate

CAS registry no.
53-21-4

Structure
Orthorhombic, $P2_12_12_1$ (19), Z = 4. The structure was refined by Gabe and Barnes [1963].

Atom positions
All atoms were in general positions 4(a). A position was not located for the hydrogen associated with the chlorine in the hydrochloride.

Lattice constants
a = 7.633(1) Å
b = 10.301(1)
c = 21.460(3)

(published values: a = 7.633(1) Å, b = 10.300(1), c = 21.459(3) [Gabe and Barnes, 1963])

CD cell: a = 10.301(1) Å, b = 21.460(3), c = 7.633(1); sp. gp. $P2_12_12_1$; a/b = 0.4800, c/b = 0.3557.

Volume
1687.3 $Å^3$

Density
(calculated) 1.338 g/cm^3
(measured) 1.342 g/cm^3 [Gabe and Barnes, 1963]

Thermal parameters
Isotropic [Gabe and Barnes, 1963]

Scattering factors
Cl^-, C^0, H^0, N^0, O^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.4587 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 0.470 for reflection with hkℓ = 002.

Additional patterns
1. PDF card 28-1609 [Owen et al., 1972]

References
Gabe, E. J. and Barnes, W. H. (1963). Acta Crystallogr. 16, 796.
International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.
Owen, J. T. R., Sithiraks, R., and Underwood, F. A. (1972). J. Ass. Off. Anal. Chem. 55, 1171.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
10.72	100	0 0 2	8.24
9.28	53	0 1 1	9.52
7.43	20	0 1 2	11.90
7.19	30	1 0 1	12.30
6.206	3	1 0 2	14.26
6.129	8	1 1 0	14.44
5.878	83	0 1 3+	15.06
5.323	35	1 1 2	16.64
5.218	8	1 0 3	16.98
5.145	24	0 2 0	17.22
5.007	9	0 2 1	17.70
4.756	64	0 1 4	18.64
4.648	55	1 1 3+	19.08
4.388	25	1 0 4	20.22
4.267	32	1 2 0	20.80
4.184	20	1 2 1	21.22
4.037	21	1 1 4	22.00
3.966	32	1 2 2	22.40
3.815	3	2 0 0	23.30
3.739	6	1 0 5	23.78
3.714	5	0 2 4	23.94
3.666	10	1 2 3	24.26
3.579	38	2 1 0	24.86
3.515	38	1 1 5	25.32
3.394	18	2 1 2	26.24
3.339	17	1 2 4	26.68
3.297	3	0 2 5	27.02
3.269	6	0 3 2	27.26
3.239	15	1 0 6	27.52
3.200	5	2 1 3	27.86
3.129	13	1 3 0	28.50
3.089	41	1 1 6	28.88
3.066	17	2 2 0	29.10
3.028	15	1 2 5+	29.48
3.006	13	1 3 2	29.70
2.976	12	2 1 4	30.00
2.947	14	2 2 2	30.30
2.868	1	1 3 3	31.16
2.819	5	2 2 3	31.72
2.741	9	1 2 6+	32.64
2.704	2	1 3 4	33.10
2.681	3	0 3 5	33.40
2.662	3	2 2 4	33.64
2.635	1	0 2 7	34.00
2.5962	2	0 1 8	34.52
2.5532	7	0 4 1+	35.12
2.5295	11	1 3 5+	35.46
2.4901	7	1 2 7+	36.04
2.4768	6	0 3 6+	36.24
2.4558	2	1 1 8+	36.56

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.4238	1	1 4 1	37.06
2.4063	2	3 1 2	37.34
2.3553	1	1 3 6	38.18
2.3283	9	2 1 7+	38.64
2.3088	6	1 4 3	38.98
2.3053	6	2 3 4+	39.04
2.2707	3	1 2 8	39.66
2.2436	2	3 1 4	40.16
2.2224	2	1 1 9+	40.56
2.1904	9	2 0 8+	41.18
2.1732	6	3 2 3	41.52
2.1682	6	2 2 7	41.62
2.1407	1	3 1 5	42.18
2.1349	1	2 4 0	42.30
2.0999	2	0 1 10+	43.04
2.0733	1	3 0 6+	43.62
2.0661	2	1 0 10	43.78
2.0439	3	3 3 0+	44.28
2.0326	5	3 1 6+	44.54
2.0188	4	2 2 8+	44.86
1.9804	4	1 5 1+	45.78
1.9618	7	2 3 7+	46.24
1.9233	3	3 2 6+	47.22
1.9172	4	0 1 11+	47.38
1.9111	4	2 4 5+	47.54
1.8968	2	1 3 9	47.92
1.8575	2	0 5 5+	49.00
1.8455	4	3 3 5+	49.34
1.8413	3	2 1 10	49.46
1.8330	2	2 4 6	49.70
1.8145	1	4 1 3+	50.24
1.8045	3	1 4 8+	50.54
1.7847	2	0 5 6+	51.14
1.7750	2	3 3 6	51.44
1.7705	2	4 1 4+	51.58
1.7572	2	2 5 3+	52.00
1.7540	2	3 4 3+	52.10
1.7379	1	2 0 11+	52.62
1.7132	3	2 1 11+	53.44
1.6973	1	4 2 4	53.98

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
10.73	100	0 0 2	8.23
9.29	54	0 1 1	9.52
7.43	20	0 1 2	11.90
7.19	31	1 0 1	12.30
6.220	2	1 0 2	14.23
6.133	7	1 1 0	14.43
5.897	50	1 1 1	15.01
5.876	51	0 1 3	15.07
5.324	37	1 1 2	16.64
5.220	5	1 0 3	16.97
5.150	25	0 2 0	17.20
5.008	9	0 2 1	17.70
4.758	69	0 1 4	18.63
4.656	35	1 1 3	19.05
4.643	30	0 2 2	19.10
4.389	27	1 0 4	20.22
4.269	34	1 2 0	20.79
4.187	20	1 2 1	21.20
4.180	1	0 2 3	21.24
4.038	22	1 1 4	21.99
3.967	36	1 2 2	22.39
3.817	2	2 0 0	23.29
3.758	1	2 0 1	23.66
3.741	5	1 0 5	23.76
3.715	4	0 2 4	23.93
3.666	11	1 2 3	24.26
3.596	4	2 0 2	24.74
3.579	40	2 1 0	24.86
3.577	1	0 0 6	24.87
3.530	3	2 1 1	25.21
3.516	42	1 1 5	25.31
3.395	20	2 1 2	26.23
3.367	1	2 0 3	26.45
3.341	19	1 2 4	26.66
3.297	2	0 2 5	27.02
3.270	5	0 3 2	27.25
3.239	17	1 0 6	27.52
3.201	5	2 1 3	27.85
3.131	14	1 3 0	28.48
3.110	2	2 0 4	28.68
3.099	12	1 3 1	28.79
3.090	40	1 1 6	28.87
3.066	15	2 2 0	29.10
3.036	7	2 2 1	29.40
3.027	11	1 2 5	29.49
3.006	13	1 3 2	29.70
2.977	12	2 1 4	29.99
2.948	14	2 2 2	30.29
2.938	6	0 2 6	30.40
2.869	1	1 3 3	31.15
2.818	7	2 2 3	31.72
2.749	4	2 1 5	32.55
2.742	1	1 1 7	32.63
2.742	8	1 2 6	32.63
2.704	2	1 3 4	33.10

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.681	3	0 3 5	33.39
2.662	3	2 2 4	33.64
2.634	1	0 2 7	34.00
2.5959	2	0 1 8	34.52
2.5752	1	0 4 0	34.81
2.5569	6	0 4 1	35.07
2.5526	3	2 3 0	35.13
2.5347	1	2 3 1	35.38
2.5298	6	2 1 6	35.45
2.5297	7	1 3 5	35.46
2.4950	3	2 2 5	35.97
2.4902	5	1 2 7	36.04
2.4833	1	2 3 2	36.14
2.4770	3	0 3 6	36.24
2.4757	2	3 0 2	36.26
2.4701	1	3 1 0	36.34
2.4577	1	1 1 8	36.53
2.4539	1	3 1 1	36.59
2.4245	1	1 4 1	37.05
2.4071	2	3 1 2	37.33
2.3560	1	1 3 6	38.17
2.3348	2	3 1 3	38.53
2.3282	5	2 1 7	38.64
2.3280	5	2 2 6	38.65
2.3216	1	0 4 4	38.76
2.3094	5	1 4 3	38.97
2.3050	3	2 3 4	39.05
2.2989	2	3 0 4	39.15
2.2714	4	1 2 8	39.65
2.2437	2	3 1 4	40.16
2.2224	2	1 1 9	40.56
2.2212	1	1 4 4	40.58
2.1946	6	2 0 8	41.10
2.1939	1	2 3 5	41.11
2.1906	5	1 3 7	41.17
2.1887	1	3 0 5	41.21
2.1733	6	3 2 3	41.52
2.1680	3	2 2 7	41.62
2.1409	1	3 1 5	42.18
2.1347	1	2 4 0	42.30
2.1009	2	0 1 10	43.02
2.0733	1	3 0 6	43.62
2.0659	2	1 0 10	43.78
2.0443	2	3 3 0	44.27
2.0372	3	1 3 8	44.43
2.0351	2	3 3 1	44.48
2.0325	3	3 1 6	44.54
2.0190	4	2 2 8	44.86
2.0081	1	3 3 2	45.11
1.9843	1	2 1 9	45.68

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.9809	1	0 2 10	45.77
1.9805	2	1 5 1	45.78
1.9797	2	0 5 3	45.80
1.9656	5	3 3 3	46.14
1.9616	6	2 3 7	46.24
1.9233	2	3 2 6	47.22
1.9174	1	1 2 10	47.37
1.9168	1	0 1 11	47.39
1.9163	1	1 5 3	47.40
1.9114	2	2 4 5	47.53
1.8971	2	1 3 9	47.91
1.8591	1	1 1 11	48.96
1.8573	1	0 5 5	49.01
1.8483	2	4 1 2	49.26
1.8456	3	3 3 5	49.34
1.8405	1	2 1 10	49.48
1.8331	2	2 4 6	49.70
1.8171	1	3 1 8	50.16
1.8149	1	4 1 3	50.23
1.8050	3	1 4 8	50.52
1.8035	2	3 4 1	50.57
1.7894	1	4 2 0	51.00
1.7852	1	0 5 6	51.12
1.7832	1	4 2 1	51.19
1.7748	1	3 3 6	51.45
1.7711	1	4 1 4	51.56
1.7574	1	2 5 3	51.99
1.7547	2	3 4 3	52.08
1.7519	1	2 4 7	52.17
1.7129	2	2 1 11	53.45
1.6975	1	4 2 4	53.97

Codeine Hydrobromide Hydrate, $C_{18}H_{22}BrNO_3 \cdot 2H_2O$

Synonyms
1. 7,8-Didehydro-4,5-α-epoxy-3-methoxy-17-methyl-morphinan-6-α-ol hydrobromide hydrate
2. Methyl morphine hydrobromide hydrate

Structure
Orthorhombic, $P2_12_12_1$ (19), Z = 4 [Lindsey and Barnes, 1955]. The structure was refined by Kartha et al. [1962]. The final R was 0.126. Intensities have been rounded to the nearer multiple of 10.

Atom positions
C, O, and N atoms were all in general positions 4(a). The Br atom was represented by 2 isotropic half-atoms separated slightly along "x". The H atom positions were not determined [Kartha et al. 1962].

Lattice constants
a = 13.090(10) Å
b = 20.826(15)
c = 6.808(5)

a/b = 0.6285
c/b = 0.3269

(published values: a = 13.089(10) Å, b = 20.825(15), c = 6.808(5) [Kartha et al.])

Volume
1856. Å^3

Density
(calculated) 1.490 g/cm^3
(measured) 1.489 [Lindsey and Barnes, 1955]

Thermal parameters
Isotropic [Kartha et al., 1962]

Scattering factors
Zero ionization [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 0.4209 \times 10^{-3}$

Additional pattern
1. PDF card 10-801 [Barnes and Lindsey, 1955]

References

Barnes, W. H. and Lindsey, J. M. (1955). Can. J. Chem. 33, 5674.

International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 211.

Kartha, G., Ahmed, F. R. and Barnes, W. H. (1962). Acta Crystallogr. 15, 326.

Lindsey, J. M. and Barnes, W. H. (1955). Acta Crystallogr. 8, 227.

Calculated Pattern (Peak heights)			
d(Å)	I	hkℓ	2Θ(°) λ - 1.540598Å
10.39	20	0 2 0	8.50
8.14	20	1 2 0	10.86
6.47	10	0 1 1	13.68
6.24	20	2 1 0	14.18
6.13	20	1 3 0	14.44
6.04	50	1 0 1	14.66
5.79	40	1 1 1	15.28
5.70	50	0 2 1	15.54
5.22	90	1 2 1+	16.98
4.83	30	1 4 0	18.34
4.72	60	2 0 1	18.80
4.60	10	2 1 1	19.28
4.55	10	1 3 1	19.48
4.27	1	3 1 0	20.78
4.13	10	0 4 1	21.48
4.02	10	3 2 0	22.08
3.942	100	1 4 1	22.54
3.904	20	2 3 1	22.76
3.616	20	3 1 1	24.60
3.551	1	0 5 1	25.06
3.496	30	2 4 1	25.46
3.466	10	3 2 1+	25.68
3.427	10	1 5 1	25.98
3.404	10	0 0 2	26.16
3.358	40	0 1 2+	26.52
3.271	10	4 0 0	27.24
3.234	10	0 2 2+	27.56
3.140	20	1 2 2	28.40
3.123	40	2 5 1+	28.56
3.056	1	0 3 2	29.20
3.002	20	3 4 1+	29.74
2.976	10	1 3 2	30.00
2.951	1	4 0 1	30.26
2.919	10	4 1 1	30.60
2.901	10	2 2 2	30.80
2.848	10	0 4 2	31.38
2.795	20	2 6 1	32.00
2.769	30	2 3 2+	32.30
2.714	20	4 3 1+	32.98
2.684	1	3 0 2	33.36
2.668	10	1 7 1	33.56
2.635	1	0 5 2	34.00
2.598	20	3 2 2+	34.50
2.566	1	4 4 1	34.94
2.553	1	1 8 0	35.12
2.517	1	2 7 1+	35.64
2.504	1	3 3 2	35.84
2.457	1	3 7 0	36.54
2.445	1	2 5 2	36.72
2.430	10	0 6 2+	36.96

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.406	1	4 5 1	37.34
2.379	10	5 2 1+	37.78
2.359	1	4 0 2	38.12
2.343	10	4 1 2	38.38
2.304	1	5 3 1	39.06
2.278	1	2 6 2+	39.52
2.255	1	3 5 2	39.94
2.235	10	3 8 0	40.32
2.208	10	1 7 2+	40.84
2.186	1	1 2 3+	41.26
2.156	1	0 3 3	41.86
2.144	1	2 0 3+	42.12
2.128	10	1 3 3+	42.44
2.123	10	3 6 2+	42.54
2.108	1	5 5 1	42.86
2.094	1	4 7 1	43.16
2.077	10	6 0 1+	43.54
2.048	1	2 3 3+	44.18
2.044	1	1 8 2+	44.28
2.038	1	5 2 2+	44.42
2.004	1	3 1 3	45.22
1.998	10	5 6 1	45.36
1.993	10	3 7 2+	45.48
1.978	1	3 2 3	45.84
1.966	1	5 7 0	46.14
1.951	1	4 6 2	46.50
1.929	1	6 4 1+	47.06
1.913	1	0 9 2	47.48
1.905	10	2 10 1+	47.70
1.894	1	1 9 2	48.00
1.889	1	5 7 1	48.14
1.878	1	1 6 3+	48.42
1.874	1	1 11 0	48.54
1.869	1	3 8 2	48.68
1.858	10	5 5 2	49.00
1.841	1	7 2 0	49.48
1.836	1	4 2 3+	49.62
1.830	1	6 1 2	49.78
1.824	1	2 6 3	49.96

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
10.41	20	0 2 0	8.48
8.15	20	1 2 0	10.85
6.55	1	2 0 0	13.52
6.47	10	0 1 1	13.67
6.24	20	2 1 0	14.17
6.13	10	1 3 0	14.43
6.04	50	1 0 1	14.65
5.80	40	1 1 1	15.26
5.70	40	0 2 1	15.54
5.22	70	1 2 1	16.96
5.21	30	0 4 0	17.02
4.84	30	1 4 0	18.32
4.76	20	2 3 0	18.62
4.72	60	2 0 1	18.79
4.60	1	2 1 1	19.27
4.56	10	1 3 1	19.47
4.30	1	2 2 1	20.65
4.27	1	3 1 0	20.78
4.14	10	0 4 1	21.47
4.07	1	2 4 0	21.79
4.02	10	3 2 0	22.07
3.969	20	1 5 0	22.38
3.944	100	1 4 1	22.53
3.902	20	2 3 1	22.77
3.618	20	3 1 1	24.59
3.553	1	0 5 1	25.04
3.514	1	2 5 0	25.33
3.496	30	2 4 1	25.46
3.471	1	0 6 0	25.64
3.464	10	3 2 1	25.69
3.429	1	1 5 1	25.96
3.404	10	0 0 2	26.16
3.359	40	0 1 2	26.51
3.355	10	1 6 0	26.55
3.344	10	3 4 0	26.63
3.273	10	4 0 0	27.23
3.254	1	1 1 2	27.39
3.247	1	3 3 1	27.45
3.236	1	0 2 2	27.55
3.233	1	4 1 0	27.57
3.141	20	1 2 2	28.39
3.123	30	2 5 1	28.56
3.122	10	4 2 0	28.57
3.056	1	0 3 2	29.20
3.009	10	1 6 1	29.66
3.002	10	3 4 1	29.74
2.989	1	2 1 2	29.87
2.976	10	1 3 2	30.00
2.960	1	4 3 0	30.17
2.949	1	4 0 1	30.28
2.920	10	4 1 1	30.59
2.900	10	2 2 2	30.80
2.849	10	0 4 2	31.37
2.838	1	4 2 1	31.50
2.796	30	2 6 1	31.98

Codeine Hydrobromide Hydrate, $C_{18}H_{22}BrNO_3 \cdot 2H_2O$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.784	1	1 4 2	32.13
2.771	10	4 4 0	32.28
2.769	20	2 3 2	32.30
2.755	10	3 5 1	32.47
2.726	1	0 7 1	32.83
2.716	10	3 6 0	32.95
2.715	10	4 3 1	32.97
2.708	10	2 7 0	33.05
2.684	1	3 0 2	33.36
2.669	1	1 7 1	33.55
2.662	1	3 1 2	33.64
2.636	1	0 5 2	33.99
2.612	1	2 4 2	34.30
2.599	10	3 2 2	34.48
2.598	10	5 1 0	34.50
2.584	1	1 5 2	34.69
2.566	1	4 4 1	34.93
2.553	1	1 8 0	35.12
2.539	1	5 2 0	35.32
2.523	1	3 6 1	35.55
2.517	1	2 7 1	35.65
2.503	1	3 3 2	35.84
2.458	1	3 7 0	36.52
2.445	1	2 5 2	36.73
2.430	1	0 6 2	36.96
2.427	1	5 1 1	37.01
2.407	1	4 5 1	37.33
2.391	1	1 8 1	37.59
2.389	1	1 6 2	37.61
2.386	1	3 4 2	37.68
2.381	1	4 6 0	37.75
2.379	10	5 2 1	37.79
2.359	1	4 0 2	38.12
2.344	10	4 1 2	38.37
2.305	1	5 3 1	39.05
2.278	1	2 6 2	39.52
2.256	1	3 5 2	39.93
2.236	10	3 8 0	40.31
2.217	1	0 2 3	40.66
2.217	1	5 5 0	40.67
2.212	1	5 4 1	40.76
2.208	1	1 7 2	40.84
2.191	1	0 9 1	41.17
2.186	1	1 2 3	41.26
2.182	1	2 9 0	41.35
2.157	1	0 3 3	41.85
2.149	1	4 4 2	42.01
2.144	1	2 0 3	42.11
2.133	10	2 1 3	42.34
2.128	10	1 3 3	42.44
2.124	1	3 8 1	42.53
2.123	1	3 6 2	42.54
2.119	1	2 7 2	42.62
2.108	1	5 5 1	42.87
2.100	1	2 2 3	43.04
2.095	1	4 7 1	43.15
2.083	1	0 10 0	43.42
2.081	1	6 3 0	43.44
2.078	1	6 0 1	43.53
2.078	1	2 9 1	43.53
2.075	1	5 0 2	43.58
2.067	1	6 1 1	43.75
2.065	1	5 1 2	43.80
2.057	1	1 10 0	43.99
2.055	1	1 4 3	44.04
2.053	1	4 5 2	44.08
2.049	1	2 3 3	44.17
2.044	1	3 9 0	44.27
2.043	1	1 8 2	44.31
2.037	1	6 2 1	44.43
2.035	1	5 2 2	44.48
2.004	1	3 1 3	45.21
1.998	1	5 6 1	45.35
1.993	10	3 7 2	45.48
1.990	1	6 3 1	45.54
1.983	1	2 4 3	45.73
1.977	1	3 2 3	45.87
1.965	1	5 7 0	46.15
1.951	1	4 6 2	46.51
1.934	1	3 3 3	46.95
1.930	1	6 4 1	47.06
1.914	1	0 9 2	47.47
1.906	1	2 5 3	47.67
1.905	10	2 10 1	47.69
1.894	1	1 9 2	48.01
1.888	1	5 7 1	48.15
1.880	1	1 6 3	48.38
1.878	1	3 4 3	48.44
1.874	1	1 11 0	48.55
1.869	1	3 8 2	48.69
1.857	10	5 5 2	49.00
1.841	1	7 2 0	49.48
1.836	1	4 2 3	49.62
1.830	1	6 1 2	49.80
1.824	1	2 6 3	49.96

Copper Arsenate (Trippkeite), $CuAs_2O_4$

Structure
Tetragonal, P4mbc (135), Z = 4. The structure was determined by Pertlik [1975].

Atom positions
[Pertlik, 1975]

4(d)	4 copper
8(g)	8 oxygen(1)
8(h)	8 oxygen(2)
8(h)	8 arsenic

Lattice constants
a = 8.592(4) Å
c = 5.573(4) [ibid.]

a/c = 0.6486

Volume
411.4 $Å^3$

Density
(calculated) 4.478 g/cm^3

Thermal parameters
Isotropic, in table 3 [Pertlik, 1975]

Scattering factors
Zero ionization [International Tables, 1962]

Scale factor (integrated intensities)
$\gamma = 1.112 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 4.16 for reflection with hkℓ = 211.

References
International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, Eng.) pp. 202, 204, 211.
Pertlik, F. (1975). Tschermak's Mineral. Petrogr. Mitt. 22, 211.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
6.07	67	1 1 0	14.58
4.30	15	2 0 0	20.66
3.841	8	2 1 0	23.14
3.401	3	2 0 1	26.18
3.162	100	2 1 1	28.20
3.038	48	2 2 0	29.38
2.786	6	0 0 2	32.10
2.717	34	3 1 0	32.94
2.532	15	1 1 2	35.42
2.4416	1	3 1 1	36.78
2.3376	33	2 0 2	38.48
2.2554	14	2 1 2	39.94
2.1914	3	3 2 1	41.16
2.1475	1	4 0 0	42.04
2.0833	2	4 1 0	43.40
2.0536	2	2 2 2	44.06
2.0044	6	4 0 1	45.20
1.9514	30	4 1 1	46.50
1.9210	7	4 2 0	47.28
1.8159	3	4 2 1	50.20
1.8118	3	3 2 2	50.32
1.7185	1	4 3 0	53.26
1.7014	10	4 0 2	53.84
1.6721	11	2 1 3	54.86
1.6381	21	3 3 2	56.10
1.6128	1	5 1 1	57.06
1.5819	1	4 2 2	58.28
1.5336	1	5 2 1+	60.30
1.5186	1	4 4 0	60.96
1.4734	8	5 3 0	63.04
1.4626	3	4 3 2	63.56
1.4420	12	5 1 2	64.58
1.4321	4	6 0 0	65.08
1.4247	3	5 3 1	65.46
1.4124	4	6 1 0	66.10
1.4053	2	4 0 3	66.48
1.3931	5	0 0 4	67.14
1.3869	9	4 1 3	67.48
1.3694	1	6 1 1	68.46
1.3579	1	1 1 4	69.12
1.3420	1	5 4 0	70.06
1.3337	2	4 4 2+	70.56
1.3197	1	6 2 1	71.42
1.3046	2	5 4 1	72.38
1.3027	2	5 3 2	72.50
1.2665	3	2 2 4	74.92
1.2599	2	6 1 2	75.38
1.2398	4	3 1 4	76.82
1.2211	5	6 2 2	78.22
1.2151	2	7 1 0+	78.68

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.2090	2	5 4 2	79.16
1.1914	1	6 4 0	80.56
1.1546	2	7 2 1+	83.70
1.1280	2	4 2 4+	86.14
1.1137	2	5 5 2+	87.52
1.1057	2	7 3 1	88.32
1.0877	1	5 4 3	90.18
1.0792	1	6 5 1	91.08
1.0705	2	2 1 5	92.04
1.0656	1	8 1 0	92.58
1.0466	2	7 4 1+	94.78
1.0458	2	7 3 2	94.88
1.0420	2	8 2 0	95.34
1.0233	1	6 5 2	97.66

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
6.08	58	1 1 0	14.57
4.30	14	2 0 0	20.66
3.842	8	2 1 0	23.13
3.402	3	2 0 1	26.17
3.163	100	2 1 1	28.19
3.038	48	2 2 0	29.38
2.787	6	0 0 2	32.10
2.717	35	3 1 0	32.94
2.533	15	1 1 2	35.41
2.4422	1	3 1 1	36.77
2.3378	35	2 0 2	38.48
2.2558	15	2 1 2	39.93
2.1911	3	3 2 1	41.17
2.1480	1	4 0 0	42.03
2.0839	2	4 1 0	43.39
2.0534	2	2 2 2	44.06
2.0043	7	4 0 1	45.20
1.9519	34	4 1 1	46.49
1.9453	1	3 1 2	46.65
1.9212	7	4 2 0	47.27
1.8163	3	4 2 1	50.19
1.8110	2	3 2 2	50.34
1.7184	1	4 3 0	53.26
1.7012	11	4 0 2	53.85
1.6725	13	2 1 3	54.85
1.6382	24	3 3 2	56.10
1.6129	1	5 1 1	57.06
1.5817	2	4 2 2	58.29
1.5339	1	5 2 1	60.29
1.5189	1	4 4 0	60.95

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.4735	10	5 3 0	63.04
1.4651	1	3 2 3	63.44
1.4626	3	4 3 2	63.56
1.4419	14	5 1 2	64.58
1.4320	4	6 0 0	65.08
1.4246	3	5 3 1	65.47
1.4125	4	6 1 0	66.10
1.4051	2	4 0 3	66.49
1.3933	6	0 0 4	67.13
1.3869	1	6 0 1	67.48
1.3867	9	4 1 3	67.49
1.3846	1	5 2 2	67.61
1.3692	1	6 1 1	68.47
1.3580	1	1 1 4	69.11
1.3418	1	5 4 0	70.07
1.3355	1	4 2 3	70.45
1.3336	2	4 4 2	70.56
1.3199	1	6 2 1	71.41
1.3046	2	5 4 1	72.38
1.3026	2	5 3 2	72.51
1.2664	4	2 2 4	74.93
1.2599	2	6 1 2	75.38
1.2398	5	3 1 4	76.83
1.2211	7	6 2 2	78.22
1.2151	1	7 1 0	78.68
1.2090	2	5 4 2	79.16
1.1915	1	6 4 0	80.56
1.1546	1	7 2 1	83.70
1.1544	1	5 3 3	83.71
1.1279	2	4 2 4	86.15
1.1138	2	5 5 2	87.51
1.1058	3	7 3 1	88.31
1.0878	1	5 4 3	90.17
1.0793	1	6 5 1	91.08
1.0705	2	2 1 5	92.04
1.0657	2	8 1 0	92.57
1.0467	1	7 4 1	94.77
1.0457	2	7 3 2	94.89
1.0419	2	8 2 0	95.34
1.0232	1	6 5 2	97.67

α-Dihydrophyllocladene, Hartite (or Bombiccite), $C_{20}H_{34}$

Synonyms
The name hartite was designated in 1841 and material called bombiccite was described later. Because of uncertainty in the chemistry, the two were not identified as the same phase until 1955 [Pellizer, 1955].

Structure
Triclinic, P1 (1), Z = 4. The structure was determined by Serantoni et al. [1978]. The natural mineral used for the determination was repeatedly dissolved and recrystallized from benzene.

Atom positions
1(a) 80 carbon
Hydrogen positions were not specified.

Lattice constants
a = 11.39(7) Å
b = 21.29(5)
c = 7.45(1)
α = 94.6(1)°
β = 101.8(2)
γ = 81.5(1)

a/b = 0.5350
c/b = 0.3499

Volume
1747. Å^3

Density
(calculated) 1.044 g/cm^3
(measured) 1.08 [Serantoni et al., 1978]

Thermal parameters
Isotropic B_i calculated from U_i given in Serantoni et al. [1978]

Scattering factors
C^0 [Cromer and Mann, 1968]

Scale factor (integrated intensities)
$\gamma = 3.162 \times 10^{-3}$

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Pellizer, R. (1955). Atti Accad. Naz. Lincei Cl. Sci. Fis. Mat. Natur. Rend. 19, 150.
Serantoni, E. F., Krajewski, A., Mongiorgi, R., Riva di Sanseverino, L. and Sheldrick, G. M. (1978). Acta Crystallogr. B34, 1311.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
21.02	5	0 1 0	4.20
10.52	35	0 2 0	8.40
8.19	3	1 2 0	10.80
7.14	7	-1 2 0	12.38
6.99	14	0 -1 1	12.66
6.64	40	-1 -1 1	13.32
6.16	40	-1 1 1	14.36
6.02	4	-1 -2 1	14.70
5.84	3	0 2 1	15.16
5.52	100	2 0 0	16.04
5.45	50	1 1 1	16.26
5.37	45	1 -1 1	16.50
5.25	9	0 4 0	16.86
5.18	13	2 2 0+	17.10
5.01	9	1 4 0+	17.70
4.92	5	-2 -1 1	18.00
4.89	3	1 -2 1+	18.14
4.64	5	-2 2 0	19.12
4.56	6	-1 3 1	19.46
4.52	6	-1 4 0	19.64
4.43	3	1 3 1+	20.04
4.33	1	-2 -3 1	20.50
4.16	3	0 4 1	21.34
4.09	3	2 4 0	21.72
4.04	1	2 0 1+	22.00
3.91	3	2 -1 1	22.72
3.89	2	-2 -4 1+	22.84
3.78	1	1 -4 1+	23.54
3.75	1	-2 3 1	23.72
3.68	2	2 -2 1+	24.16
3.61	1	2 3 1+	24.64
3.58	2	-2 4 0+	24.88
3.55	1	-3 1 0	25.08
3.48	2	1 6 0	25.60
3.39	1	0 2 2+	26.30
3.37	1	-1 5 1+	26.40
3.36	1	-2 0 2	26.54
3.33	2	-3 2 0+	26.78
3.22	1	3 4 0+	27.68
3.16	2	-1 -4 2+	28.22
3.13	1	-1 3 2+	28.48
3.06	4	3 1 1	29.14
3.01	2	-2 -4 2+	29.68
2.98	1	3 -1 1	29.92
2.92	1	0 4 2+	30.56
2.88	3	-1 4 2+	30.98
2.76	2	4 0 0+	32.38
2.72	1	-4 -3 1+	32.88
2.64	1	1 8 0	33.96
2.60	1	-2 -6 2	34.50

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.54	1	3 -4 1	35.26
2.426	1	4 0 1+	37.02
2.387	2	4 -1 1+	37.66
2.353	1	-4 -4 2+	38.22
2.301	1	-1 -9 1+	39.12
2.281	1	-2 6 2+	39.48
2.259	1	0 -9 1+	39.88
2.214	1	-1 -5 3+	40.72
2.200	1	-2 3 3+	41.00
2.162	1	-4 -6 2+	41.74
2.119	1	1 10 0+	42.64
2.091	2	-3 -5 3+	43.24

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
21.03	5	0 1 0	4.20
10.51	35	0 2 0	8.40
8.19	3	1 2 0	10.80
7.15	6	-1 2 0	12.37
6.99	14	0 -1 1	12.65
6.77	1	0 1 1	13.06
6.65	45	-1 -1 1	13.30
6.17	45	-1 1 1	14.35
6.14	2	0 -2 1	14.42
6.02	3	-1 -2 1	14.70
5.85	2	0 2 1	15.14
5.60	5	1 0 1	15.82
5.53	5	2 1 0	16.02
5.52	100	2 0 0	16.03
5.45	45	1 1 1	16.25
5.37	45	1 -1 1	16.49
5.35	1	-1 2 1	16.55
5.26	6	0 4 0	16.85
5.20	2	-1 -3 1	17.05
5.19	6	2 2 0	17.08
5.19	2	0 -3 1	17.08
5.17	3	-2 1 0	17.12
5.02	5	1 4 0	17.67
5.00	5	1 2 1	17.72
4.93	4	-2 -1 1	17.99
4.88	1	-2 0 1	18.15
4.88	2	1 -2 1	18.15
4.65	1	2 3 0	19.05
4.64	5	-2 2 0	19.11
4.60	1	-2 1 1	19.26
4.56	6	-1 3 1	19.44
4.52	6	-1 4 0	19.64
4.44	2	1 3 1	20.00
4.43	1	-1 -4 1	20.04
4.33	1	-2 -3 1	20.48
4.16	3	0 4 1	21.33
4.09	3	2 4 0	21.69
4.08	1	-2 3 0	21.77
4.04	1	2 0 1	22.00
3.91	3	2 -1 1	22.70
3.89	1	-2 -4 1	22.85
3.78	1	1 -4 1	23.52
3.75	1	-2 3 1	23.73
3.68	1	2 -2 1	24.14
3.64	1	0 0 2	24.43
3.61	1	2 3 1	24.65
3.58	2	-2 4 0	24.88
3.55	1	-3 1 0	25.08
3.48	3	1 6 0	25.59
3.36	1	-2 0 2	26.53
3.34	1	-3 2 0	26.68
3.32	1	-2 -2 2	26.79
3.16	1	-1 -4 2	28.20
3.13	1	-1 3 2	28.45
3.08	1	-2 2 2	28.93
3.06	5	3 1 1	29.14
3.05	1	3 0 1	29.21
3.01	1	-2 -4 2	29.64
2.98	1	3 -1 1	29.91
2.92	1	0 4 2	30.55
2.90	1	3 3 1	30.83
2.89	3	-1 4 2	30.97
2.76	1	-3 4 1	32.35
2.76	1	4 0 0	32.39
2.64	1	1 8 0	33.95
2.60	1	-2 -6 2	34.50
2.54	1	3 -4 1	35.26
2.387	1	-3 4 2	37.65
2.386	1	4 -1 1	37.66
2.317	1	4 -2 1	38.84
2.281	1	-2 6 2	39.47
2.214	1	-1 -5 3	40.71
2.200	1	-2 3 3	41.00
2.091	1	-3 -5 3	43.24

(-)-Ephedrine Hydrochloride, $C_{10}H_{16}ClNO$

Synonyms
1. Biophedrin
2. Ephedral
3. Sanedrine

CAS registry no.
877-36-1

Structure
Monoclinic, $P2_1$ (4), Z = 2. The structure was determined by Phillips [1954]. Bergin [1971] refined the structure using 3-dimensional data.

Atom positions
All atoms were in general positions 2(a) [Bergin, 1971].

Lattice constants
Bergin [1971]
a = 12.671(3) Å
b = 6.090(4)
c = 7.301(2)
β = 102.11(8)°

a/b = 2.0806
c/b = 1.1989

Volume
550.9 $Å^3$

Density
(calculated) 1.216 g/cm^3

Thermal parameters
Anisotropic [Bergin, 1971]

Scattering factors
Zero ionization [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.6728 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 0.962 for reflection with hkℓ = 011.

Additional patterns
1. PDF card 5-0263 [E. Lilly and Co., Indianapolis, IN]
2. PDF card 24-1735 [Institute of Physics, University College, Cardiff, Wales]

References

Bergin, R. (1971). Acta Crystallogr. B27, 381.

International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Phillips, D. C. (1954). Acta Crystallogr. 7, 159.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
12.37	9	1 0 0	7.14
7.13	17	0 0 1	12.40
6.84	45	-1 0 1	12.94
6.19	4	2 0 0	14.30
5.68	9	1 0 1	15.58
5.46	15	1 1 0	16.22
4.629	100	0 1 1	19.16
4.544	21	-1 1 1	19.52
4.341	18	2 1 0	20.44
4.130	25	3 0 0	21.50
3.976	4	-2 1 1	22.34
3.952	4	-3 0 1	22.48
3.636	2	-1 0 2	24.46
3.567	27	0 0 2	24.94
3.488	10	2 1 1	25.52
3.417	35	3 1 0+	26.06
3.314	9	-3 1 1	26.88
3.123	5	-1 1 2	28.56
3.079	20	0 1 2	28.98
3.046	3	0 2 0	29.30
2.980	18	-2 1 2	29.96
2.957	6	1 2 0	30.20
2.893	9	3 1 1	30.88
2.868	13	1 1 2	31.16
2.781	5	-1 2 1	32.16
2.754	9	-4 1 1+	32.48
2.733	3	2 2 0	32.74
2.715	6	-3 1 2	32.96
2.684	4	1 2 1	33.36
2.635	5	-2 2 1	34.00
2.577	2	2 1 2	34.78
2.477	4	2 2 1	36.24
2.426	4	4 1 1	37.02
2.413	5	-3 2 1+	37.24
2.396	1	-2 0 3	37.50
2.379	4	0 0 3	37.78
2.335	1	-1 2 2	38.52
2.317	1	-5 1 1+	38.84
2.295	1	5 1 0	39.22
2.273	6	-2 2 2	39.62
2.260	3	-1 1 3	39.86
2.252	2	1 0 3	40.00
2.230	5	-2 1 3+	40.42
2.171	2	4 2 0	41.56
2.148	3	-3 2 2	42.02
2.134	3	-3 1 3	42.32
2.129	3	4 0 2+	42.42
2.105	3	-6 0 1	42.94
2.079	2	2 2 2	43.50
2.009	1	4 1 2	45.10

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.004	2	1 3 0	45.22
1.998	2	4 2 1+	45.36
1.990	1	-6 1 1+	45.54
1.975	1	-6 0 2	45.90
1.955	2	6 1 0	46.40
1.947	1	-1 3 1	46.62
1.929	1	2 3 0	47.08
1.912	1	3 2 2+	47.52
1.901	1	-1 2 3	47.82
1.881	4	6 0 1+	48.36
1.876	3	0 2 3	48.48
1.840	1	-5 1 3	49.50
1.832	1	2 3 1	49.72
1.821	2	3 3 0+	50.06
1.810	1	1 2 3+	50.38
1.744	2	-2 1 4+	52.42
1.731	1	-6 2 1	52.84
1.721	2	4 0 3+	53.18
1.713	2	0 1 4	53.46
1.696	1	-4 3 1+	54.02
1.683	1	-6 1 3	54.46
1.652	1	1 1 4+	55.58
1.578	1	-5 3 1	58.42
1.562	2	-2 2 4+	59.10

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
12.39	8	1 0 0	7.13
7.14	15	0 0 1	12.39
6.84	43	-1 0 1	12.94
6.19	3	2 0 0	14.29
5.69	8	1 0 1	15.56
5.47	14	1 1 0	16.20
4.633	100	0 1 1	19.14
4.547	18	-1 1 1	19.50
4.343	18	2 1 0	20.43
4.158	8	1 1 1	21.35
4.130	24	3 0 0	21.50
3.979	3	-2 1 1	22.32
3.952	3	-3 0 1	22.48
3.639	1	-1 0 2	24.44
3.569	28	0 0 2	24.93
3.489	10	2 1 1	25.51
3.418	14	-2 0 2	26.05
3.418	23	3 1 0	26.05
3.315	9	-3 1 1	26.87
3.124	4	-1 1 2	28.55
3.097	4	4 0 0	28.80
3.088	1	-4 0 1	28.89
3.079	20	0 1 2	28.97
3.045	2	0 2 0	29.31
2.981	20	-2 1 2	29.95
2.957	5	1 2 0	30.20
2.893	9	3 1 1	30.88
2.869	14	1 1 2	31.15
2.782	5	-1 2 1	32.15
2.761	3	4 1 0	32.40
2.754	7	-4 1 1	32.49
2.733	2	2 2 0	32.75
2.715	6	-3 1 2	32.96
2.685	4	1 2 1	33.35
2.646	2	4 0 1	33.85
2.635	5	-2 2 1	34.00
2.578	2	2 1 2	34.77
2.477	4	2 2 1	36.24
2.433	1	-1 0 3	36.91
2.427	4	4 1 1	37.01
2.413	1	-4 1 2	37.23
2.412	5	-3 2 1	37.25
2.396	1	-2 0 3	37.51
2.380	4	0 0 3	37.78
2.335	1	-1 2 2	38.52
2.295	1	5 1 0	39.22
2.279	1	-3 0 3	39.51
2.274	6	-2 2 2	39.61
2.260	2	-1 1 3	39.86
2.251	1	1 0 3	40.02
2.234	3	3 2 1	40.34
2.230	3	-2 1 3	40.42
2.171	2	4 2 0	41.56
2.149	3	-3 2 2	42.01
2.134	2	-3 1 3	42.31
2.129	1	4 0 2	42.43
2.105	3	-6 0 1	42.93
2.079	3	2 2 2	43.50
2.009	1	4 1 2	45.08
2.003	1	1 3 0	45.23
1.997	1	4 2 1	45.37
1.989	1	-6 1 1	45.56
1.976	1	-6 0 2	45.89
1.955	3	6 1 0	46.40
1.946	1	-1 3 1	46.64
1.929	1	2 3 0	47.07
1.901	1	-1 2 3	47.81
1.883	2	-2 2 3	48.30
1.881	2	6 0 1	48.35
1.880	1	-6 1 2	48.39

(-)-Ephedrine Hydrochloride, $C_{10}H_{16}ClNO$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.875	2	0 2 3	48.52
1.840	1	-5 1 3	49.49
1.832	1	2 3 1	49.72
1.825	1	-3 2 3	49.95
1.822	1	3 3 0	50.03
1.820	1	-5 2 2	50.07
1.810	1	1 2 3	50.37
1.745	1	-2 3 2	52.38
1.743	1	-2 1 4	52.45
1.731	1	-6 2 1	52.83
1.722	1	1 3 2	53.14
1.721	1	4 0 3	53.19
1.713	2	0 1 4	53.46
1.696	1	-4 3 1	54.02
1.684	2	-6 1 3	54.45
1.578	1	-5 3 1	58.43
1.564	1	-5 1 4	59.02
1.562	2	-2 2 4	59.10

Haloperidol, $C_{21}H_{23}ClFNO_2$

Synonyms
1. Haldol
2. Serenase
3. 4-(4-hydroxy-4-p-chlorphenylpiperidino)4'-fluorobutyrophenone

CAS registry no.
52-86-8

Structure
Monoclinic, $P2_1/c$ (14), Z = 4. The structure was refined by Reed and Schaefer [1973].

Atom positions
All atoms were in general positions 4(e). The "x" parameter for carbon(7) was used as 0.0838. No hydrogen positions were listed in the reference.

Lattice constants

a = 7.816(5) Å
b = 8.996(6)
c = 28.346(20)
β = 106.34°

(published values: a = 7.816(5)Å, b = 8.995(6), c = 28.344(20), β = 106.34(4)° [Reed and Schaefer, 1973])

CD cell: a = 27.202, b = 8.996, c = 7.816, β = 90.33°, space group $P2_1/n$; a/b = 3.0237, c/b = 0.8688

Volume
1912.6 $Å^3$

Density
(calculated) 1.305 g/cm^3
(measured) 1.23 g/cm^3 [Reed and Schaefer, 1973]

Thermal parameters
Anisotropic [Reed and Schaefer, 1973]

Scattering factors
Zero ionization [International Tables, 1962]

Scale factor (integrated intensities)

$\gamma = 1.271 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 1.29 for reflection with hkℓ = $\bar{1}15$.

References

International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.
Reed, L. L. and Schaefer, J. P. (1973). Acta Crystallogr. B29, 1886.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
8.53	2	0 1 1	10.36
7.49	10	1 0 0+	11.80
6.79	1	0 0 4	13.02
6.38	3	0 1 3	13.86
5.93	19	-1 0 4+	14.94
5.76	5	-1 1 2+	15.36
5.41	6	1 1 1+	16.36
4.946	2	-1 1 4+	17.92
4.653	3	0 1 5	19.06
4.467	100	-1 1 5	19.86
4.044	1	0 1 6	21.96
3.897	13	-1 2 1	22.80
3.751	3	0 2 4+	23.70
3.584	11	-1 2 4+	24.82
3.464	1	2 1 0+	25.70
3.396	7	-2 0 6+	26.22
3.339	2	-2 1 5	26.68
3.177	6	-2 1 6	28.06
3.000	6	-2 1 7	29.76
2.986	5	2 1 3+	29.90
2.951	2	-1 1 9+	30.26
2.934	3	-2 2 3+	30.44
2.881	3	2 2 0+	31.02
2.808	4	-2 2 5+	31.84
2.784	3	1 3 0+	32.12
2.745	2	1 2 6+	32.60
2.711	2	-2 2 6	33.02
2.641	1	-2 1 9	33.92
2.592	1	-2 2 7+	34.58
2.508	1	0 2 9	35.78
2.491	1	-1 3 6+	36.02
2.474	2	-1 1 11+	36.28
2.464	3	-3 1 5+	36.44
2.370	1	-2 3 1+	37.94
2.354	1	-2 2 9+	38.20
2.345	2	-2 3 4+	38.36
2.248	1	-2 3 6+	40.08
2.226	1	2 0 8+	40.50
2.129	1	0 3 9	42.42
2.119	1	-1 1 13	42.64
2.113	1	1 1 11+	42.76
2.103	1	-1 4 4+	42.98
2.010	3	3 1 5+	45.08
1.955	1	2 0 10+	46.40
1.947	2	-3 3 5+	46.62
1.907	1	-2 4 5	47.66
1.873	1	-2 3 11+	48.58

Calculated Pattern (Integrated)			
d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
8.54	2	0 1 1	10.35
7.52	1	-1 0 2	11.75
7.50	3	0 1 2	11.79
7.50	6	1 0 0	11.79
6.80	1	0 0 4	13.01
6.39	3	0 1 3	13.86
5.94	15	-1 0 4	14.91
5.90	5	1 0 2	15.00
5.90	9	-1 1 1	15.00
5.77	3	-1 1 2	15.34
5.76	2	1 1 0	15.37
5.42	3	0 1 4	16.33
5.42	2	-1 1 3	16.34
5.40	3	1 1 1	16.39
4.955	1	-1 1 4	17.89
4.935	1	1 1 2	17.96
4.655	2	0 1 5	19.05
4.534	2	0 0 6	19.57
4.498	55	0 2 0	19.72
4.477	2	-1 0 6	19.81
4.466	100	-1 1 5	19.86
4.048	1	0 1 6	21.94
3.908	1	-2 0 2	22.74
3.899	13	-1 2 1	22.79
3.762	1	-2 0 4	23.63
3.752	2	0 2 4	23.70
3.603	4	-1 1 7	24.69
3.585	9	-1 2 4	24.81
3.578	3	1 2 2	24.87
3.400	1	0 0 8	26.19
3.397	6	-2 0 6	26.21
3.386	2	-1 2 5	26.30
3.378	1	1 2 3	26.36
3.339	2	-2 1 5	26.67
3.178	6	-2 1 6	28.06
3.165	2	1 2 4	28.18
3.000	7	-2 1 7	29.75
2.986	3	2 1 3	29.90
2.981	2	0 3 1	29.95
2.969	2	-2 0 8	30.08
2.941	1	0 2 7	30.37
2.934	2	-2 2 3	30.44
2.886	1	-2 2 4	30.96
2.880	2	2 2 0	31.02
2.813	2	1 0 8	31.78
2.809	2	-2 2 5	31.83
2.786	1	-1 3 2	32.11
2.784	3	1 3 0	32.12
2.756	1	-1 2 8	32.46
2.748	1	1 2 6	32.56
2.711	2	-2 2 6	33.02
2.642	1	-2 1 9	33.91
2.598	1	-2 2 7	34.49
2.509	1	0 2 9	35.76
2.474	2	-1 1 11	36.28
2.464	2	-3 1 5	36.44
2.369	1	-2 3 1	37.95
2.345	2	-2 3 4	38.36
2.248	1	-2 3 6	40.08
2.226	1	2 0 8	40.48
2.129	1	0 3 9	42.43
2.119	1	-1 1 13	42.63
2.103	1	-1 4 4	42.97
2.010	2	3 1 5	45.07
2.007	1	1 4 4	45.13
1.956	1	2 0 10	46.39
1.948	1	-3 3 5	46.59
1.945	1	-2 4 3	46.67
1.907	1	-2 4 5	47.65

Imipramine Hydrochloride, $C_{19}H_{25}ClN_2$

Synonyms
1. 5-(3-Dimethylaminopropyl)-10,11-dihydro-5H-dibenz[b,f]azepine hydrochloride
2. Berkomine
3. Tofranil
4. Deprinol

Structure
Monoclinic, $P2_1$ (14), Z = 8. The structure was refined by Post et al. [1975].

Atom positions
All atoms were in general positions 4(e).

Lattice constants
a = 11.304(3) Å
b = 29.229(8)
c = 14.283(3)
β = 130.91(1)°

(published values: a = 11.303(3) Å, b = 29.227(8), c = 14.282(3), β = 130.91(1)° [Post et al., 1975])

CD cell: a = 11.304(1), b = 29.229(8), c = 10.969(3), β = 100.24(1)°; sp. gp. $P2_1/n$; a/b = 0.3867, c/b = 0.3753

Volume
3566.5 Å^3

Density
(calculated) 1.180 g/cm^3
(measured) 1.18 g/cm^3 [Post et al., 1975]

Thermal parameters
For hydrogen atoms, overall isotropic B = 7.26, converted from U_{iso} = 0.092 Å^2. For all other atoms, isotropic B_i were estimated from U_{ij} for individual atoms.

Scattering factors
Zero ionization [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.2872 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 0.285 for reflection with hkℓ = 060.

Additional pattern
1. PDF card 27-1765 [de Leenheer and Heyndrickx, 1971]. The primary reference indicates that the powder data are for the HCl derivative; apparently the name and formula on the card are in error.

References

International Tables for X-ray Crystallography III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.
de Leenheer, A. and Heyndrickx, A. (1971). J. Ass. Off. Anal. Chem. 54, 625.
Post, M. L., Kennard, O. and Horn, A. S. (1975). Acta Crystallogr. B31, 1008.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2Θ(°) λ - 1.540598Å
14.62	8	0 2 0	6.04
10.11	78	0 1 1	8.74
8.53	86	1 0 0	10.36
8.20	14	1 1 0	10.78
7.36	30	1 2 0+	12.02
7.23	77	0 3 1	12.24
7.13	46	-1 0 2	12.40
6.932	13	-1 1 2	12.76
6.104	2	-1 4 1	14.50
5.757	8	-1 3 2	15.38
5.549	47	1 4 0	15.96
5.460	97	-2 1 2	16.22
5.304	6	0 1 2	16.70
5.187	21	-2 2 2+	17.08
5.018	71	-2 2 1	17.66
4.870	100	0 6 0	18.20
4.721	7	0 3 2	18.78
4.609	10	1 3 1	19.24
4.562	11	-2 1 3	19.44
4.432	40	-2 4 2+	20.02
4.267	56	2 0 0+	20.80
4.172	35	-2 3 3	21.28
4.100	56	2 2 0+	21.66
4.030	7	-2 5 2	22.04
3.942	10	-2 5 1	22.54
3.907	17	2 3 0+	22.74
3.751	50	1 7 0	23.70
3.714	36	-3 0 2	23.94
3.684	39	2 4 0+	24.14
3.666	39	-2 6 2	24.26
3.613	24	0 6 2+	24.62
3.567	53	-2 0 4	24.94
3.545	24	-2 1 4	25.10
3.466	54	-2 2 4+	25.68
3.388	5	1 3 2	26.28
3.324	30	-1 6 3+	26.80
3.290	10	-2 7 1+	27.08
3.250	30	-1 8 2+	27.42
3.207	27	-2 4 4	27.80
3.164	10	-3 3 1	28.18
3.129	10	-3 5 3+	28.50
3.089	5	-1 3 4	28.88
3.074	6	1 5 2+	29.02
3.054	9	-2 8 2	29.22
3.028	5	0 8 2	29.48
2.974	5	-1 4 4	30.02
2.955	8	-1 9 2+	30.22
2.923	4	0 10 0	30.56
2.904	3	-3 5 1+	30.76
2.895	3	-3 5 4+	30.86

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.866	5	-2 8 3	31.18
2.847	7	3 0 0+	31.40
2.826	4	-1 10 1	31.64
2.819	5	-3 1 5	31.72
2.776	7	2 8 0+	32.22
2.731	12	-4 2 4+	32.76
2.727	12	0 7 3+	32.82
2.704	11	-4 3 3+	33.10
2.699	11	0 0 4	33.16
2.673	3	-4 3 4	33.50
2.653	12	0 2 4+	33.76
2.630	5	-4 2 2	34.06
2.617	5	2 0 2+	34.24
2.602	8	-3 7 4+	34.44
2.579	4	0 11 1+	34.76
2.552	3	1 10 1+	35.14
2.548	3	-3 5 5	35.20
2.531	5	0 4 4+	35.44
2.512	2	-4 5 4	35.72
2.498	2	-4 3 5	35.92
2.491	2	-1 11 2	36.02
2.478	1	1 5 3	36.22
2.458	2	3 6 0	36.52
2.431	3	-4 5 2+	36.94
2.411	2	1 9 2+	37.26
2.379	8	-2 11 1+	37.78
2.360	6	0 6 4	38.10
2.354	6	3 7 0	38.20
2.345	4	-4 6 2	38.36
2.325	4	3 3 1+	38.70
2.300	4	-1 9 4+	39.14
2.296	4	-4 4 1	39.20
2.283	2	-4 6 5+	39.44
2.274	2	1 10 2+	39.60
2.261	3	-5 0 4+	39.84
2.247	3	3 8 0+	40.10
2.233	3	-5 2 4+	40.36
2.215	4	3 5 1+	40.70
2.203	6	-1 13 1+	40.94
2.175	4	-5 2 3+	41.48
2.170	4	1 2 4+	41.58
2.158	2	-4 8 2+	41.82
2.135	6	4 0 0+	42.30
2.121	6	-2 9 5+	42.60
2.107	3	-5 0 6+	42.88
2.084	7	-2 13 2+	43.38
2.079	6	-3 11 4+	43.50
2.072	5	-2 13 1	43.64
2.059	3	-5 1 2	43.94
2.050	4	-5 6 4+	44.14

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.044	4	-5 2 2	44.28
2.039	3	2 9 2+	44.40
2.021	4	-4 9 5+	44.80
2.013	4	-4 2 7+	45.00
1.999	2	1 6 4+	45.32
1.987	2	3 3 2+	45.62
1.955	3	4 6 0+	46.40
1.945	3	-5 7 3+	46.66
1.938	3	-3 11 5+	46.84
1.922	3	-3 13 2+	47.26
1.918	4	0 15 1+	47.36
1.907	3	0 13 3+	47.64
1.902	2	-2 14 3+	47.78
1.898	2	-1 14 3	47.88

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
14.61	7	0 2 0	6.04
10.40	3	-1 1 1	8.50
10.13	73	0 1 1	8.73
8.54	81	1 0 0	10.35
8.20	12	1 1 0	10.78
7.38	19	1 2 0	11.99
7.33	10	-1 3 1	12.07
7.23	66	0 3 1	12.23
7.14	34	-1 0 2	12.39
6.934	10	-1 1 2	12.76
6.107	1	-1 4 1	14.49
5.758	7	-1 3 2	15.38
5.553	40	1 4 0	15.95
5.464	93	-2 1 2	16.21
5.397	6	0 0 2	16.41
5.307	2	0 1 2	16.69
5.198	15	-2 2 2	17.04
5.175	8	-1 5 1	17.12
5.140	2	0 5 1	17.24
5.106	4	-1 4 2	17.35
5.063	13	0 2 2	17.50
5.021	67	-2 2 1	17.65
4.872	100	0 6 0	18.20
4.824	5	1 5 0	18.38
4.721	5	0 3 2	18.78
4.612	8	1 3 1	19.23
4.564	9	-2 1 3	19.43
4.523	1	-1 5 2	19.61
4.494	5	-1 1 3	19.74
4.462	25	-1 6 1	19.88

Imipramine Hydrochloride, $C_{19}H_{25}ClN_2$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
4.440	20	0 6 1	19.98
4.426	21	-2 4 2	20.05
4.406	2	-2 2 3	20.14
4.315	9	-2 4 1	20.57
4.271	44	2 0 0	20.78
4.256	20	1 4 1	20.86
4.232	15	1 6 0	20.98
4.227	6	2 1 0	21.00
4.175	32	-2 3 3	21.26
4.121	23	-1 3 3	21.54
4.100	49	2 2 0	21.66
4.029	4	-2 5 2	22.04
3.945	7	-2 5 1	22.52
3.912	13	2 3 0	22.71
3.909	1	-1 7 1	22.73
3.900	2	1 5 1	22.78
3.894	4	0 7 1	22.82
3.751	50	1 7 0	23.70
3.716	30	-3 0 2	23.93
3.688	15	2 4 0	24.11
3.686	14	-3 1 2	24.12
3.678	5	-3 1 3	24.18
3.665	30	-2 6 2	24.27
3.625	5	-2 5 3	24.54
3.616	14	0 6 2	24.60
3.604	6	-1 7 2	24.68
3.601	2	-2 6 1	24.70
3.594	1	-3 2 3	24.75
3.590	5	-1 5 3	24.78
3.590	2	1 1 2	24.78
3.569	51	-2 0 4	24.93
3.543	16	-2 1 4	25.12
3.511	1	1 2 2	25.35
3.471	9	-1 8 1	25.64
3.467	32	-2 2 4	25.67
3.465	13	-3 3 3	25.69
3.461	8	0 8 1	25.72
3.449	1	2 5 0	25.81
3.391	4	1 3 2	26.26
3.375	1	0 3 3	26.38
3.339	10	-2 7 2	26.67
3.330	3	-3 0 4	26.75
3.325	6	-3 1 1	26.79
3.325	20	-1 6 3	26.79
3.308	3	-3 1 4	26.93
3.307	1	-3 4 3	26.94
3.291	5	-2 7 1	27.07
3.280	2	2 1 1	27.17
3.262	3	-3 2 1	27.32
3.258	8	-1 0 4	27.35

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
3.252	14	-1 8 2	27.40
3.246	12	-3 2 4	27.45
3.212	3	2 6 0	27.75
3.207	24	-2 4 4	27.80
3.180	1	-1 2 4	28.04
3.165	9	-3 3 1	28.17
3.136	3	-3 5 2	28.44
3.131	6	-3 5 3	28.48
3.126	1	2 3 1	28.53
3.118	3	-1 9 1	28.61
3.110	2	0 9 1	28.68
3.098	1	-2 7 3	28.79
3.090	2	-1 3 4	28.87
3.076	1	-3 7 3	29.01
3.076	4	1 5 2	29.01
3.064	1	0 5 3	29.12
3.054	8	-2 8 2	29.22
3.043	2	-3 4 1	29.33
3.030	1	-3 4 4	29.46
3.026	2	0 8 2	29.50
3.017	1	-2 8 1	29.59
2.976	5	-1 4 4	30.01
2.956	5	-1 9 2	30.21
2.954	3	-3 6 2	30.23
2.923	4	0 10 0	30.56
2.904	2	-3 5 1	30.76
2.894	1	0 6 3	30.87
2.893	1	-3 5 4	30.88
2.866	4	-2 8 3	31.18
2.848	4	3 0 0	31.39
2.846	3	-1 5 4	31.41
2.834	1	3 1 0	31.54
2.827	2	-1 10 1	31.62
2.817	3	-3 1 5	31.74
2.795	2	3 2 0	31.99
2.779	1	-3 2 5	32.19
2.776	2	2 8 0	32.21
2.776	2	-3 7 2	32.22
2.776	1	-2 9 1	32.22
2.752	1	-2 2 5	32.51
2.749	1	-3 6 4	32.55
2.734	4	1 7 2	32.73
2.732	6	-4 2 4	32.75
2.726	4	0 7 3	32.83
2.718	2	-3 3 5	32.93
2.713	1	-2 7 4	32.99
2.706	6	-4 3 3	33.08
2.705	2	-1 10 2	33.09
2.699	6	0 0 4	33.17
2.674	1	-4 3 4	33.48

Imipramine Hydrochloride, $C_{19}H_{25}ClN_2$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.657	4	-2 9 3	33.70
2.654	9	0 2 4	33.75
2.653	1	3 4 0	33.75
2.639	1	-3 4 5	33.94
2.630	3	-4 2 2	34.07
2.618	3	2 0 2	34.23
2.617	1	-2 4 5	34.24
2.603	3	-3 7 4	34.42
2.602	2	-3 8 3	34.43
2.601	1	0 3 4	34.46
2.599	2	-4 4 4	34.48
2.580	2	0 11 1	34.74
2.577	1	2 2 2	34.79
2.552	1	1 10 1	35.14
2.547	1	-3 5 5	35.20
2.537	2	1 11 0	35.35
2.531	3	0 4 4	35.43
2.527	1	-2 5 5	35.50
2.511	2	-4 5 4	35.73
2.498	1	-4 3 5	35.92
2.490	1	-1 11 2	36.04
2.478	1	1 5 3	36.22
2.458	1	3 6 0	36.52
2.438	1	-4 6 3	36.83
2.431	2	-4 5 2	36.95
2.416	1	1 9 2	37.18
2.411	1	0 9 3	37.27
2.386	2	1 6 3	37.67
2.384	1	-1 4 5	37.71
2.379	5	-2 11 1	37.78
2.361	6	0 6 4	38.09
2.353	3	3 7 0	38.22
2.344	2	-4 6 2	38.38
2.325	2	-3 9 4	38.70
2.325	2	3 3 1	38.70
2.315	1	2 9 1	38.87
2.311	1	-3 3 6	38.93
2.306	1	2 6 2	39.03
2.300	2	-1 9 4	39.13
2.296	1	-4 4 1	39.21
2.283	1	-4 6 5	39.44
2.273	1	1 10 2	39.61
2.262	1	-3 4 6	39.81
2.260	2	-5 0 4	39.86
2.248	1	-4 3 6	40.08
2.246	1	3 8 0	40.11
2.233	2	-5 2 4	40.35
2.215	2	3 5 1	40.70
2.204	4	-1 13 1	40.92
2.201	2	0 13 1	40.97

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.199	1	-5 2 5	41.00
2.176	2	-1 10 4	41.47
2.175	2	-5 2 3	41.49
2.169	1	1 2 4	41.60
2.140	1	1 3 4	42.20
2.138	1	-3 6 6	42.24
2.136	3	4 0 0	42.28
2.134	2	-3 9 5	42.32
2.122	3	-2 9 5	42.58
2.120	3	-2 5 6	42.62
2.106	1	-5 0 6	42.91
2.093	2	-4 7 1	43.20
2.088	1	0 14 0	43.30
2.085	2	-5 2 6	43.37
2.085	5	-2 13 2	43.37
2.077	2	-3 11 4	43.54
2.077	1	3 7 1	43.54
2.073	3	-2 13 1	43.64
2.064	2	-4 9 2	43.83
2.058	1	-5 1 2	43.95
2.050	3	-5 6 4	44.14
2.043	2	-5 2 2	44.30
2.022	2	-4 9 5	44.78
2.022	1	-4 7 6	44.80
2.013	2	-4 2 7	45.00
2.012	1	-2 12 4	45.02
1.987	1	3 3 2	45.63
1.956	2	4 6 0	46.38
1.955	1	-2 14 2	46.42
1.946	1	-5 7 3	46.64
1.945	1	-3 4 7	46.66
1.943	1	3 11 0	46.72
1.937	1	-3 11 5	46.86
1.924	1	-3 13 2	47.21
1.922	1	-5 2 7	47.25
1.918	1	0 15 1	47.37
1.907	1	0 13 3	47.66
1.897	1	-1 14 3	47.90

Morphine Hydrochloride Hydrate, $C_{17}H_{20}ClNO_3 \cdot 3H_2O$

Synonyms
1. (-)-7,8-Didehydro-4,5-α-epoxy-17-methylmorphinan-3,6-α-diol hydrochloride hydrate
2. Morphine Chlorhydrate
3. Morphine Chloride Hydrate

Structure
Orthorhombic, $P2_12_12_1$ (19), Z = 4. The structure was determined by Gylbert [1973].

Atom positions
All atoms were in general positions 4(a). Bond lengths were calculated and indicated that the "z" coordinate of atom C3 should be 0.0935. That value was used in these calculations.

Lattice constants
a = 13.020(7) Å
b = 20.751(10)
c = 6.941(4)

a/b = 0.6274
c/b = 0.3345

(published values: a = 13.019(7) Å, b = 20.750(10), c = 6.941(4) [Gylbert, 1973]

Volume
1875.3 $Å^3$

Density
(calculated) 1.331 g/cm^3
(measured) 1.310 g/cm^3 [Gylbert, 1973]

Thermal parameters
Isotropic. For the hydrogen atoms, overall B = 3.0 [Gylbert, 1973]. For other atoms, isotropic B_i were estimated from β_{ij} for individual atoms.

Scattering factors
C^0, H^0, Cl^0, N^0, O^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.4275 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 0.421, for reflection with hkℓ = 020.

Additional patterns
1. PDF card 10-798 [Barnes and Lindsey, 1955]

References

Barnes, W. H. and Lindsey, J. M. (1955). Can. J. Chem. 33, 565.
Gylbert, L. (1973). Acta Crystallogr. B29, 1630.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
11.02	6	1 1 0	8.02
10.37	89	0 2 0	8.52
8.11	40	1 2 0	10.90
6.11	100	1 0 1+	14.48
5.870	29	1 1 1	15.08
5.764	84	0 2 1	15.36
5.273	24	1 2 1	16.80
5.187	17	0 4 0	17.08
4.897	20	0 3 1	18.10
4.818	18	1 4 0	18.40
4.746	35	2 0 1+	18.68
4.624	11	2 1 1	19.18
4.586	6	1 3 1	19.34
4.316	15	2 2 1	20.56
4.153	15	0 4 1	21.38
4.055	9	2 4 0	21.90
3.955	82	1 4 1	22.46
3.914	26	2 3 1	22.70
3.675	6	3 3 0	24.20
3.622	12	3 1 1	24.56
3.559	2	0 5 1	25.00
3.501	32	2 4 1+	25.42
3.469	16	0 0 2+	25.66
3.422	29	0 1 2	26.02
3.351	7	1 0 2	26.58
3.329	7	3 4 0	26.76
3.293	3	0 2 2	27.06
3.191	14	1 2 2	27.94
3.123	33	2 5 1	28.56
3.104	15	0 3 2+	28.74
3.054	3	2 6 0	29.22
3.012	16	1 3 2+	29.64
3.002	15	3 5 0	29.74
2.938	13	2 2 2+	30.40
2.884	5	0 4 2	30.98
2.833	1	4 2 1	31.56
2.800	9	2 3 2	31.94
2.753	9	3 5 1	32.50
2.727	2	0 7 1	32.82
2.711	2	3 0 2	33.02
2.688	3	3 1 2	33.30
2.668	4	1 7 1+	33.56
2.636	2	2 4 2	33.98
2.623	2	3 2 2	34.16
2.608	3	1 5 2	34.36
2.560	2	4 5 0	35.02
2.514	12	2 7 1+	35.68
2.464	4	2 5 2	36.44
2.448	5	3 7 0+	36.68
2.421	6	5 1 1	37.10

Morphine Hydrochloride Hydrate, $C_{17}H_{20}ClNO_2 \cdot 3H_2O$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.403	7	3 4 2+	37.40
2.389	3	1 8 1	37.62
2.373	4	5 2 1	37.88
2.359	4	4 1 2	38.12
2.314	2	4 2 2	38.88
2.299	3	5 3 1	39.16
2.293	4	2 6 2	39.26
2.270	8	3 5 2	39.68
2.244	6	4 6 1+	40.16
2.226	7	3 8 0	40.50
2.221	6	1 7 2	40.58
2.207	2	5 4 1	40.86
2.193	2	0 3 3	41.12
2.188	2	0 9 1	41.22
2.163	8	1 3 3+	41.72
2.133	3	3 6 2+	42.34
2.121	1	3 8 1	42.60
2.102	2	5 5 1	43.00
2.085	4	1 4 3+	43.36
2.080	4	2 3 3+	43.48
2.074	4	2 9 1+	43.60
2.061	5	6 1 1	43.90
2.041	1	3 0 3	44.34
2.032	4	3 1 3+	44.56
2.010	2	2 4 3	45.08
2.000	6	3 7 2+	45.30
1.996	4	5 6 1	45.40
1.965	1	1 10 1	46.16
1.958	3	4 6 2+	46.34
1.947	1	4 8 1	46.60
1.933	3	5 4 2+	46.98
1.923	2	6 4 1+	47.22
1.902	2	1 6 3+	47.78
1.883	1	5 7 1+	48.30
1.873	2	3 8 2	48.56
1.867	4	1 11 0	48.74
1.862	5	5 5 2	48.88
1.853	2	4 7 2+	49.12
1.844	1	2 6 3	49.38
1.838	2	5 8 0+	49.56
1.832	2	3 5 3+	49.72
1.807	2	3 10 1+	50.46
1.803	2	1 11 1	50.58
1.790	1	7 1 1	50.98
1.785	1	5 6 2	51.14
1.777	2	5 8 1+	51.38
1.765	1	1 10 2	51.76
1.757	1	3 9 2+	52.02
1.729	2	5 0 3+	52.90
1.726	2	0 8 3	53.00

Calculated Pattern (Integrated)			
d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
11.03	5	1 1 0	8.01
10.38	100	0 2 0	8.52
8.11	46	1 2 0	10.89
6.21	4	2 1 0	14.25
6.12	66	1 0 1	14.45
6.11	59	1 3 0	14.49
5.874	28	1 1 1	15.07
5.769	98	0 2 1	15.35
5.275	28	1 2 1	16.80
5.188	18	0 4 0	17.08
4.900	23	0 3 1	18.09
4.819	19	1 4 0	18.39
4.748	33	2 0 1	18.67
4.741	9	2 3 0	18.70
4.629	12	2 1 1	19.16
4.586	5	1 3 1	19.34
4.318	18	2 2 1	20.55
4.155	18	0 4 1	21.37
4.057	10	2 4 0	21.89
3.959	86	1 4 1	22.44
3.954	18	1 5 0	22.47
3.915	26	2 3 1	22.70
3.680	1	3 0 1	24.17
3.676	7	3 3 0	24.19
3.623	15	3 1 1	24.55
3.562	1	0 5 1	24.98
3.503	30	2 4 1	25.41
3.500	11	2 5 0	25.43
3.470	10	0 0 2	25.65
3.468	6	3 2 1	25.67
3.458	1	0 6 0	25.74
3.436	7	1 5 1	25.91
3.423	34	0 1 2	26.01
3.353	7	1 0 2	26.56
3.343	2	1 6 0	26.65
3.329	6	3 4 0	26.76
3.310	2	1 1 2	26.91
3.291	3	0 2 2	27.07
3.216	3	4 1 0	27.72
3.191	18	1 2 2	27.94
3.125	43	2 5 1	28.54
3.106	5	4 2 0	28.72
3.102	10	0 3 2	28.76
3.054	2	2 6 0	29.22
3.030	5	2 1 2	29.46
3.017	13	1 3 2	29.58
3.012	7	1 6 1	29.64
3.001	2	3 4 1	29.74
2.999	12	3 5 0	29.76
2.947	5	4 0 1	30.30

Morphine Hydrochloride Hydrate, $C_{17}H_{20}ClNO_3 \cdot 3H_2O$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.945	3	4 3 0	30.32
2.937	12	2 2 2	30.41
2.918	2	4 1 1	30.62
2.890	1	1 7 0	30.91
2.885	6	0 4 2	30.98
2.835	1	4 2 1	31.53
2.816	3	1 4 2	31.75
2.800	11	2 3 2	31.93
2.757	1	4 4 0	32.45
2.753	11	3 5 1	32.49
2.726	2	0 7 1	32.83
2.710	2	3 0 2	33.02
2.698	1	2 7 0	33.18
2.688	3	3 1 2	33.31
2.668	5	1 7 1	33.56
2.662	1	0 5 2	33.64
2.637	2	2 4 2	33.97
2.622	3	3 2 2	34.16
2.608	3	1 5 2	34.35
2.561	3	4 5 0	35.01
2.524	5	3 3 2	35.54
2.520	6	3 6 1	35.60
2.515	10	2 7 1	35.68
2.464	5	2 5 2	36.43
2.450	2	0 6 2	36.65
2.448	5	3 7 0	36.68
2.421	7	5 1 1	37.10
2.403	3	4 5 1	37.40
2.402	6	3 4 2	37.40
2.389	3	1 8 1	37.63
2.373	5	5 2 1	37.88
2.359	5	4 1 2	38.12
2.314	3	4 2 2	38.88
2.299	3	5 3 1	39.14
2.293	3	2 6 2	39.26
2.276	1	2 8 1	39.56
2.269	11	3 5 2	39.68
2.246	3	4 3 2	40.12
2.243	6	4 6 1	40.17
2.227	7	3 8 0	40.48
2.225	1	1 2 3	40.51
2.221	3	1 7 2	40.59
2.207	2	5 4 1	40.86
2.194	1	0 3 3	41.11
2.188	1	0 9 1	41.22
2.173	1	2 9 0	41.52
2.168	5	2 1 3	41.62
2.164	8	1 3 3	41.71
2.133	1	2 2 3	42.33
2.133	3	3 6 2	42.33

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.120	1	3 8 1	42.61
2.102	3	5 5 1	42.99
2.090	1	4 7 1	43.25
2.086	3	1 4 3	43.35
2.083	1	5 0 2	43.41
2.079	1	2 3 3	43.49
2.074	2	2 9 1	43.60
2.061	6	6 1 1	43.90
2.061	1	4 5 2	43.90
2.042	1	3 0 3	44.33
2.032	3	3 1 3	44.56
2.031	2	6 2 1	44.58
2.029	1	4 8 0	44.63
2.021	1	0 5 3	44.81
2.010	2	2 4 3	45.07
2.003	1	3 2 3	45.23
2.000	6	3 7 2	45.30
1.993	1	5 6 1	45.48
1.965	1	1 10 1	46.15
1.958	1	3 3 3	46.33
1.957	2	4 6 2	46.35
1.947	1	4 8 1	46.61
1.933	3	5 4 2	46.97
1.930	1	2 5 3	47.05
1.924	1	6 4 1	47.21
1.923	1	0 6 3	47.23
1.902	2	1 6 3	47.77
1.883	1	5 7 1	48.29
1.874	2	3 8 2	48.54
1.867	4	1 11 0	48.74
1.862	4	5 5 2	48.89
1.853	1	4 7 2	49.12
1.844	1	2 6 3	49.38
1.838	1	5 8 0	49.56
1.832	1	3 5 3	49.73
1.812	1	2 11 0	50.32
1.808	2	3 10 1	50.45
1.803	1	1 11 1	50.59
1.790	1	7 1 1	50.98
1.784	1	5 6 2	51.15
1.777	1	5 8 1	51.39
1.765	1	1 10 2	51.77
1.756	1	3 9 2	52.03
1.730	1	5 0 3	52.89
1.727	2	0 8 3	52.99

Naloxone Hydrochloride Hydrate, $C_{19}H_{22}ClNO_4 \cdot 2H_2O$

Synonyms
1. 17-Allyl-4,5-epoxy-3,14-dihydroxy-morphinan-6-one hydrochloride hydrate
2. (-)-N-Allyl-7,8-dihydro-14-hydroxy-morphinone hydrochloride hydrate

Structure
Orthorhombic, $P2_12_12_1$ (19), Z = 4. The structure was refined in 1975 by Sime et al., and in 1974 by Karle.

Atom positions
All atoms were in the general positions 4(a) given by Sime et al. [1975]. The "x" parameter for C(15) appeared to be in error, and the value 0.1908 was used instead, in these calculations.

Lattice constants
a = 7.833(3) Å
b = 13.186(5)
c = 18.570(5)

(published values: a = 7.833(3) Å, b = 13.185(5), c = 18.569(5) [Sime et al.,1975])

CD cell: a = 13.185(5), b = 18.570(5), c = 7.833(3); sp. gp. = $P2_12_12_1$; a/b = 0.7101, c/b = 0.4218

Volume
1918.0 $Å^3$

Density
(calculated) 1.385 g/cm^3
(measured) 1.35 g/cm^3 [Sime et al.]

Thermal parameters
Isotropic. For hydrogen: overall B = 4.0 and for other atoms, B_i was estimated from B_{ij} for individual atoms.

Scattering factors
H^0 [International Tables, 1962]
All other atoms, zero ionization, from Cromer and Mann [1968]. The chlorine atoms were corrected for dispersion [Cromer and Liberman, 1970].

Scale factors (integrated intensities)
$\gamma = 1.196 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 1.13 for the reflection with hkℓ = 101.

References
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.
Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.), p. 202.
Karle, I. L. (1974). Acta Crystallogr. B30, 1682.
Sime, R. L., Forehand, R. and Sime, R. J. (1975). Acta Crystallogr. B31, 2326.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
10.75	6	0 1 1	8.22
9.28	2	0 0 2	9.52
7.58	13	0 1 2	11.66
7.21	100	1 0 1	12.26
6.73	11	1 1 0	13.14
6.59	27	0 2 0	13.42
6.33	26	1 1 1	13.98
5.45	27	1 1 2	16.26
5.37	6	0 2 2	16.48
4.87	12	1 2 1	18.22
4.55	5	1 1 3	19.48
4.51	2	0 2 3	19.66
4.43	11	1 2 2	20.02
4.28	2	0 3 1	20.76
3.911	5	1 2 3+	22.72
3.831	11	1 3 0	23.20
3.751	23	1 3 1+	23.70
3.678	3	2 1 1	24.18
3.607	6	2 0 2	24.66
3.542	11	1 3 2	25.12
3.480	4	2 1 2	25.58
3.414	2	1 2 4	26.08
3.356	7	1 0 5+	26.54
3.312	18	2 2 1	26.90
3.252	5	1 3 3+	27.40
3.209	2	2 1 3	27.78
3.164	1	2 2 2	28.18
3.038	10	1 4 0	29.38
2.992	9	1 2 5+	29.84
2.955	6	1 3 4+	30.22
2.917	3	2 1 4+	30.62
2.912	3	0 4 3	30.68
2.888	3	1 4 2	30.94
2.790	6	2 3 2	32.06
2.727	4	2 2 4+	32.82
2.687	2	0 4 4	33.32
2.667	1	1 3 5	33.58
2.638	6	1 2 6+	33.96
2.560	2	3 1 0	35.02
2.542	1	1 4 4+	35.28
2.521	1	2 4 0	35.58
2.498	4	2 4 1	33.92
2.468	5	3 1 2+	36.38
2.426	2	0 5 3+	37.02
2.408	2	1 3 6+	37.32
2.348	4	1 2 7+	38.30
2.278	2	2 2 6	39.52
2.257	2	0 4 6+	39.92
2.226	1	1 0 8	40.50
2.201	2	1 5 4	40.98

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.182	2	3 3 2+	41.34
2.173	1	2 5 1	41.52
2.151	1	3 2 4	41.96
2.129	2	2 5 2	42.42
2.110	2	3 3 3+	42.82
2.086	1	2 4 5+	43.34
2.063	2	1 6 2+	43.86
2.047	1	3 4 0	44.22
1.999	3	3 4 2+	45.34
1.973	1	3 1 6+	45.96
1.944	1	1 5 6+	46.68
1.921	1	3 3 5+	47.28
1.910	2	1 2 9+	47.58
1.896	1	4 1 2	47.94
1.892	1	0 6 5	48.06
1.868	1	0 3 9+	48.72
1.855	1	3 5 0	49.06
1.839	2	4 2 2+	49.52

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
10.75	6	0 1 1	8.22
10.75	6	0 -1 -1	8.22
9.28	2	0 0 2	9.52
9.28	2	0 0 -2	9.52
7.59	12	0 1 2	11.65
7.59	12	0 -1 -2	11.65
7.22	100	1 0 1	12.25
7.22	100	-1 0 -1	12.25
6.73	9	1 1 0	13.14
6.73	9	-1 -1 0	13.14
6.59	27	0 2 0	13.42
6.59	27	0 -2 0	13.42
6.33	26	1 1 1	13.98
6.33	27	-1 -1 -1	13.98
5.45	28	1 1 2	16.25
5.45	28	-1 -1 -2	16.25
5.38	4	0 2 2	16.48
5.38	4	0 -2 -2	16.48
4.87	13	1 2 1	18.21
4.87	12	-1 -2 -1	18.21
4.56	5	1 1 3	19.46
4.56	6	-1 -1 -3	19.46
4.51	1	0 2 3	19.66
4.51	1	0 -2 -3	19.66
4.43	12	1 2 2	20.02
4.43	11	-1 -2 -2	20.02
4.28	2	0 3 1	20.75
4.28	2	0 -3 -1	20.75
3.916	3	2 0 0	22.69
3.916	3	-2 0 0	22.69
3.910	3	1 2 3	22.72
3.910	3	-1 -2 -3	22.72
3.833	11	1 3 0	23.19
3.833	11	-1 -3 0	23.19
3.822	2	1 1 4	23.25
3.822	1	-1 -1 -4	23.25
3.754	11	2 1 0	23.68
3.754	11	-2 -1 0	23.68
3.754	14	1 3 1	23.68
3.754	15	-1 -3 -1	23.68
3.680	3	2 1 1	24.17
3.680	3	-2 -1 -1	24.17
3.609	6	2 0 2	24.65
3.609	6	-2 0 -2	24.65
3.543	12	1 3 2	25.11
3.543	12	-1 -3 -2	25.11
3.481	4	2 1 2	25.57
3.481	4	-2 -1 -2	25.57
3.416	2	1 2 4	26.07
3.416	2	-1 -2 -4	26.07
3.367	3	2 2 0	26.45
3.367	3	-2 -2 0	26.45
3.356	5	1 0 5	26.54
3.356	5	-1 0 -5	26.54
3.313	19	2 2 1	26.89
3.313	18	-2 -2 -1	26.89
3.310	2	2 0 3	26.92
3.310	2	-2 0 -3	26.92
3.259	3	1 3 3	27.34
3.259	3	-1 -3 -3	27.34
3.252	3	1 1 5	27.40
3.252	3	-1 -1 -5	27.40
3.246	1	0 4 1	27.46
3.246	1	0 -4 -1	27.46
3.236	1	0 2 5	27.54
3.236	1	0 -2 -5	27.54
3.210	2	2 1 3	27.77
3.210	2	-2 -1 -3	27.77
3.165	1	2 2 2	28.17
3.165	1	-2 -2 -2	28.17
3.038	12	1 4 0	29.37
3.038	12	-1 -4 0	29.37
2.994	4	2 0 4	29.82
2.994	4	-2 0 -4	29.82
2.991	6	1 2 5	29.85

Naloxone Hydrochloride Hydrate, $C_{19}H_{22}ClNO_4 \cdot 2H_2O$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.991	6	-1 -2 -5	29.85
2.958	3	2 2 3	30.19
2.958	3	-2 -2 -3	30.19
2.956	4	1 3 4	30.21
2.956	4	-1 -3 -4	30.21
2.924	1	2 3 0	30.55
2.924	1	-2 -3 0	30.55
2.919	2	2 1 4	30.60
2.919	2	-2 -1 -4	30.60
2.910	2	0 4 3	30.70
2.910	2	0 -4 -3	30.70
2.888	2	1 4 2	30.94
2.888	2	-1 -4 -2	30.94
2.812	1	1 1 6	31.79
2.812	1	-1 -1 -6	31.79
2.802	2	0 2 6	31.92
2.802	2	0 -2 -6	31.92
2.789	7	2 3 2	32.07
2.789	7	-2 -3 -2	32.07
2.728	2	1 4 3	32.81
2.728	2	-1 -4 -3	32.81
2.726	3	2 2 4	32.83
2.726	3	-2 -2 -4	32.83
2.688	2	0 4 4	33.31
2.688	2	0 -4 -4	33.31
2.667	1	1 3 5	33.57
2.667	1	-1 -3 -5	33.57
2.644	1	2 3 3	33.88
2.644	1	-2 -3 -3	33.88
2.640	1	2 1 5	33.92
2.640	1	-2 -1 -5	33.92
2.638	6	1 2 6	33.96
2.638	6	-1 -2 -6	33.96
2.561	2	3 1 0	35.01
2.561	2	-3 -1 0	35.01
2.542	1	1 4 4	35.27
2.542	1	-1 -4 -4	35.27
2.522	1	2 4 0	35.57
2.522	1	-2 -4 0	35.57
2.499	4	2 4 1	35.91
2.499	4	-2 -4 -1	35.91
2.474	1	2 3 4	36.28
2.474	1	-2 -3 -4	36.28
2.469	3	3 1 2	36.36
2.469	3	-3 -1 -2	36.36
2.465	2	0 4 5	36.41
2.465	2	0 -4 -5	36.41
2.428	1	3 2 0	37.00
2.428	1	-3 -2 0	37.00
2.426	1	0 5 3	37.02
2.426	1	0 -5 -3	37.02
2.408	1	1 3 6	37.31
2.408	1	-1 -3 -6	37.31
2.349	2	3 2 2	38.29
2.349	2	-3 -2 -2	38.29
2.348	3	1 2 7	38.30
2.348	3	-1 -2 -7	38.30
2.279	2	2 2 6	39.52
2.279	2	-2 -2 -6	39.52
2.256	2	0 4 6	39.92
2.256	2	0 -4 -6	39.92
2.226	1	1 0 8	40.50
2.226	1	-1 0 -8	40.50
2.201	2	1 5 4	40.98
2.201	2	-1 -5 -4	40.98
2.182	1	3 3 2	41.35
2.182	1	-3 -3 -2	41.35
2.172	1	2 5 1	41.53
2.172	1	-2 -5 -1	41.53
2.151	1	3 2 4	41.96
2.151	1	-3 -2 -4	41.96
2.129	2	2 5 2	42.42
2.129	2	-2 -5 -2	42.42
2.110	2	3 3 3	42.82
2.110	2	-3 -3 -3	42.82
2.086	1	2 4 5	43.33
2.086	1	-2 -4 -5	43.33
2.063	1	1 6 2	43.85
2.063	1	-1 -6 -2	43.85
2.047	1	3 4 0	44.22
2.047	1	-3 -4 0	44.22
1.999	2	3 4 2	45.34
1.999	2	-3 -4 -2	45.34
1.944	1	1 5 6	46.67
1.944	1	-1 -5 -6	46.67
1.910	1	1 2 9	47.58
1.910	1	-1 -2 -9	47.58
1.896	1	4 1 2	47.94
1.896	1	-4 -1 -2	47.94
1.891	1	0 6 5	48.07
1.891	1	0 -6 -5	48.07
1.840	1	4 2 2	49.50
1.840	1	-4 -2 -2	49.50
1.839	1	0 1 10	49.53
1.839	1	0 -1-10	49.53

Palladium Selenium (Palladseite), $Pd_{17}Se_{15}$

Structure
Cubic, Z = 2. The space group Pm3m was used for the structure determination by Geller [1962] and for the powder pattern here. The x-ray data did not eliminate uncertainty about the space group which could also be $P\bar{4}3m$ or P432 [Geller, 1962].

Atom positions

24(m)	24 palladium
12(j)	12 selenium
12(i)	12 selenium
6(f)	6 selenium
6(e)	6 palladium
3(d)	3 palladium
1(b)	1 palladium

Lattice constants
a = 10.607(3) Å

(published value: a = 10.606(3) Å [Geller, 1962]).

Volume
1193.4 $Å^3$

Density
(calculated) 8.330 g/cm^3

Thermal parameters
Isotropic, Table 2 [Geller, 1962]

Scattering factors
Pd^0, Se^0 [Thomas and Umeda, 1957], corrected for dispersion [Cromer and Liberman, 1970]

Scale factor (integrated intensities)
$\gamma = 0.4090 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 4.11 for reflection with hkℓ = 440.

References
Cromer, D. T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891.
Geller, S. (1962). Acta Crystallogr. 15, 713.
Thomas, L. H. and Umeda, K. (1957). J. Chem. Phys. 26, 293.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
5.30	5	2 0 0	16.72
4.741	3	2 1 0	18.70
4.329	1	2 1 1	20.50
3.748	4	2 2 0	23.72
3.534	4	2 2 1	25.18
3.353	44	3 1 0	26.56
3.198	91	3 1 1	27.88
3.062	3	2 2 2	29.14
2.942	18	3 2 0	30.36
2.834	52	3 2 1	31.54
2.572	64	4 1 0+	34.86
2.499	32	4 1 1	35.90
2.4327	26	3 3 1	36.92
2.3720	25	4 2 0	37.90
2.3145	20	4 2 1	38.88
2.1215	11	4 3 0+	42.58
2.0797	12	4 3 1+	43.48
2.0413	79	3 3 3	44.34
1.9365	1	5 2 1	46.88
1.8748	100	4 4 0	48.52
1.8462	3	5 2 2	49.32
1.8193	9	4 3 3+	50.10
1.7925	1	5 3 1	50.90
1.7679	36	6 0 0	51.66
1.7435	4	6 1 0	52.44
1.7203	16	5 3 2+	53.20
1.6772	6	6 2 0	54.68
1.6566	17	5 4 0+	55.42
1.6365	15	5 4 1	56.16
1.6175	3	5 3 3	56.88
1.5814	5	5 4 2+	58.30
1.5309	2	4 4 4	60.42
1.5155	2	7 0 0	61.10
1.5000	5	7 1 0+	61.80
1.4853	1	5 5 1	62.48
1.4709	5	6 4 0	63.16
1.4569	2	6 4 1	63.84
1.4049	2	5 4 4+	66.50
1.3927	3	7 3 0	67.16
1.3807	25	7 3 1	67.82
1.3579	5	6 4 3	69.12
1.3470	6	7 3 2+	69.76
1.3258	9	8 0 0	71.04
1.3156	3	7 4 0+	71.68
1.3055	9	5 5 4+	72.32
1.2959	12	7 3 3	72.94
1.2862	12	6 4 4	73.58
1.2770	5	7 4 2+	74.20
1.2677	1	6 5 3	74.84
1.2501	9	6 6 0	76.08

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.2415	1	8 3 0+	76.70
1.2331	6	7 4 3	77.32
1.2248	5	7 5 1	77.94
1.2167	1	6 6 2	78.56
1.1858	3	8 4 0	81.02
1.1786	3	7 4 4+	81.62
1.1713	4	9 1 0	82.24
1.1643	1	9 1 1+	82.84
1.1573	5	8 4 2	83.46
1.1505	3	7 6 0	84.06
1.1437	7	7 6 1+	84.68

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
5.30	4	2 0 0	16.70
4.744	2	2 1 0	18.69
4.330	1	2 1 1	20.49
3.750	3	2 2 0	23.71
3.536	3	2 2 1	25.17
3.354	38	3 1 0	26.55
3.198	79	3 1 1	27.87
3.062	3	2 2 2	29.14
2.942	16	3 2 0	30.36
2.835	47	3 2 1	31.53
2.573	44	4 1 0	34.85
2.573	16	3 2 2	34.85
2.500	29	4 1 1	35.89
2.4334	24	3 3 1	36.91
2.3718	23	4 2 0	37.90
2.3146	19	4 2 1	38.88
2.1214	5	4 3 0	42.58
2.1214	5	5 0 0	42.58
2.0802	5	5 1 0	43.47
2.0802	6	4 3 1	43.47
2.0413	6	5 1 1	44.34
2.0413	71	3 3 3	44.34
1.9366	1	5 2 1	46.88
1.8751	100	4 4 0	48.51
1.8464	2	5 2 2	49.31
1.8191	2	5 3 0	50.11
1.8191	7	4 3 3	50.11
1.7929	1	5 3 1	50.89
1.7678	36	6 0 0	51.66
1.7438	4	6 1 0	52.43
1.7207	6	6 1 1	53.19
1.7207	10	5 3 2	53.19
1.6771	6	6 2 0	54.68
1.6565	7	5 4 0	55.42
1.6565	3	6 2 1	55.42
1.6565	7	4 4 3	55.42
1.6367	15	5 4 1	56.15
1.6176	3	5 3 3	56.88
1.5812	3	5 4 2	58.31
1.5812	2	6 3 0	58.31
1.5310	2	4 4 4	60.42
1.5153	2	7 0 0	61.11
1.5001	3	7 1 0	61.80
1.5001	2	5 5 0	61.80
1.4853	1	5 5 1	62.48
1.4709	5	6 4 0	63.16
1.4570	2	6 4 1	63.83
1.4049	2	5 4 4	66.50
1.3928	2	7 3 0	67.16
1.3809	27	7 3 1	67.81
1.3581	5	6 4 3	69.11
1.3471	3	7 3 2	69.76
1.3471	3	6 5 1	69.76
1.3259	10	8 0 0	71.04
1.3156	3	7 4 0	71.68
1.3056	3	7 4 1	72.31
1.3056	1	8 1 1	72.31
1.3056	6	5 5 4	72.31
1.2959	13	7 3 3	72.94
1.2863	13	6 4 4	73.58
1.2769	4	7 4 2	74.20
1.2769	1	8 2 1	74.20
1.2678	1	6 5 3	74.83
1.2500	9	6 6 0	76.08
1.2330	6	7 4 3	77.32
1.2248	5	7 5 1	77.94
1.2167	1	6 6 2	78.56
1.1859	3	8 4 0	81.02
1.1786	2	7 4 4	81.63
1.1713	4	9 1 0	82.24
1.1643	1	9 1 1	82.85
1.1573	5	8 4 2	83.46
1.1505	3	7 6 0	84.06
1.1438	4	7 6 1	84.67
1.1438	3	9 2 1	84.67

Phencyclidine Hydrochloride, $C_{17}H_{26}ClN$

Synonyms
1. 1-(1-Phenylcyclohexyl) piperidine hydrochloride
2. Sernyl hydrochloride
3. Sernylan
4. PCP hydrochloride

CAS registry no.
956-90-1

Structure
Monoclinic, $P2_1/c$ (14), Z = 4. The structure was determined by Argos et al. [1970].

Atom positions
All atoms were in general positions [ibid.]

Lattice constants
a = 8.881(10) Å
b = 13.867(20)
c = 13.099(10)
β = 104.55(16)°

(published values: a = 8.881(10), b = 13.866(20), c = 13.098(10), β = 104°33'(10') [Argos et al., 1970])

CD cell: a = 13.099(10) Å, b = 13.867(20), c = 8.881(10), β = 104.55(16)°; sp. gp. $P2_1/a$; a/b = 0.9446; c/b = 0.6404

Volume
1561.4 $Å^3$

Density
(calculated) 1.190 g/cm^3
(measured) 1.190(4) [Argos et al., 1970]

Thermal parameters
Isotropic B_i, estimated from β_{ij} for individual atoms.

Scattering factors
Zero ionization [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.6975 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 0.751 for reflection with hkℓ = 021.

Additional pattern
1. Folen [1975]

References

Argos, P., Barr, R. E., and Weber, A. H. (1970). Acta Crystallogr. B26, 53.
Folen, V. A. (1975). J. Forensic Sci. 20, 348.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
9.34	16	0 1 1	9.46
8.58	57	1 0 0	10.30
6.93	6	0 2 0	12.76
6.34	15	0 0 2	13.96
6.08	100	0 2 1	14.56
5.80	15	1 1 1	15.26
5.76	22	0 1 2	15.36
5.39	2	-1 1 2	16.44
5.27	14	-1 2 1	16.80
4.68	18	0 2 2	18.96
4.47	19	-1 2 2	19.84
4.34	22	0 3 1	20.44
4.30	25	2 0 0	20.66
4.10	9	2 1 0	21.64
4.05	38	-1 1 3+	21.92
3.90	18	-2 1 2	22.80
3.82	26	1 2 2	23.26
3.73	11	-2 2 1	23.86
3.65	26	2 1 1+	24.34
3.62	23	-1 3 2+	24.54
3.36	2	1 1 3	26.52
3.33	11	2 2 1	26.78
3.25	3	1 3 2	27.40
3.21	3	1 4 0	27.74
3.16	24	-1 1 4+	28.18
3.12	23	0 3 3+	28.60
3.05	3	1 4 1	29.28
2.942	4	-1 2 4	30.36
2.895	9	-3 1 1+	30.86
2.864	7	-2 1 4+	31.20
2.773	4	1 3 3+	32.26
2.722	6	-2 4 1+	32.88
2.696	3	-2 2 4+	33.20
2.682	5	-1 4 3	33.38
2.624	7	-1 5 1	34.14
2.608	4	3 1 1	34.36
2.541	1	0 5 2+	35.30
2.510	1	2 2 3	35.74
2.493	3	-3 3 1+	36.00
2.455	3	-2 4 3+	36.58
2.368	2	1 3 4+	37.96
2.361	2	3 1 2	38.08
2.329	4	-2 2 5+	38.62
2.277	2	-1 3 5+	39.54
2.251	5	1 1 5	40.02
2.223	3	-1 6 1+	40.54
2.180	2	-2 3 5+	41.38
2.166	2	1 2 5+	41.66
2.149	2	4 0 0+	42.00
2.126	5	2 4 3	42.48

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.123	5	4 1 0+	42.54
2.107	3	-4 2 1+	42.88
2.053	4	4 2 0+	44.08
2.026	4	-2 2 6+	44.70
2.022	4	0 2 6	44.78
2.015	5	4 1 1+	44.96
1.995	2	-4 3 1+	45.42
1.980	2	-3 3 5	45.78
1.948	2	4 3 0+	46.58
1.942	2	1 0 6	46.74
1.930	5	1 7 0+	47.04
1.926	4	-1 7 1+	47.16
1.891	2	0 7 2+	48.08
1.870	2	1 2 6+	48.64
1.846	1	-2 5 5+	49.34
1.818	1	3 4 3	50.14
1.805	1	-1 2 7+	50.52
1.794	1	0 7 3+	50.86
1.762	1	1 5 5+	51.86
1.756	2	2 7 1+	52.04
1.750	1	-4 3 5	52.22
1.719	1	2 1 6+	53.24
1.700	2	-5 2 3+	53.88
1.696	2	1 4 6+	54.02
1.689	2	-5 1 4+	54.28
1.672	1	0 8 2	54.86
1.662	1	-1 8 2	55.22
1.646	1	-1 4 7	55.82
1.641	1	1 2 7+	56.00
1.622	1	-1 1 8+	56.70
1.614	1	-5 1 5+	57.00
1.586	1	1 3 7+	58.10
1.563	1	-3 0 8+	59.06

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
9.36	16	0 1 1	9.44
8.60	57	1 0 0	10.28
7.01	1	-1 1 1	12.62
6.93	6	0 2 0	12.76
6.34	14	0 0 2	13.96
6.08	100	0 2 1	14.55
5.85	1	-1 0 2	15.13
5.82	10	1 1 1	15.22
5.77	19	0 1 2	15.36
5.39	1	-1 1 2	16.43
5.27	14	-1 2 1	16.80
4.71	3	1 2 1	18.84
4.68	17	0 2 2	18.95
4.47	19	-1 2 2	19.84
4.35	1	1 1 2	20.40
4.34	21	0 3 1	20.43
4.30	25	2 0 0	20.65
4.11	7	2 1 0	21.63
4.06	10	-2 0 2	21.86
4.05	33	-1 1 3	21.91
4.04	1	0 1 3	21.97
4.02	4	-1 3 1	22.11
3.90	19	-2 1 2	22.79
3.82	28	1 2 2	23.25
3.75	1	1 3 1	23.72
3.73	11	-2 2 1	23.85
3.66	16	2 1 1	24.32
3.65	11	2 2 0	24.35
3.63	17	-1 3 2	24.52
3.62	9	-1 2 3	24.60
3.61	1	0 2 3	24.65
3.36	2	1 1 3	26.50
3.33	12	2 2 1	26.78
3.25	3	1 3 2	27.39
3.22	2	1 4 0	27.72
3.19	4	-1 4 1	27.96
3.17	7	0 0 4	28.13
3.17	20	-1 1 4	28.17
3.15	9	2 3 0	28.33
3.12	9	2 1 2	28.58
3.12	15	0 3 3	28.60
3.11	3	-2 2 3	28.66
3.05	2	1 4 1	29.27
2.943	5	-1 2 4	30.34
2.908	2	2 2 2	30.72
2.899	5	-3 0 2	30.82
2.894	5	-3 1 1	30.87
2.865	4	3 0 0	31.19
2.863	4	-2 1 4	31.21
2.781	2	-2 3 3	32.16
2.772	3	1 3 3	32.27
2.728	4	-2 4 1	32.80
2.722	3	-3 2 1	32.88
2.709	2	0 5 1	33.04
2.696	2	-2 2 4	33.20
2.683	4	-1 4 3	33.37
2.639	2	1 5 0	33.94
2.637	1	-2 4 2	33.97
2.625	8	-1 5 1	34.13
2.614	1	0 3 4	34.28
2.608	3	3 1 1	34.36
2.541	1	0 5 2	35.30
2.511	1	2 2 3	35.73
2.494	1	0 1 5	35.97
2.492	3	-3 3 1	36.01

Phencyclidine Hydrochloride, $C_{17}H_{26}ClN$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.457	2	-2 4 3	36.54
2.454	1	-3 0 4	36.58
2.449	1	-1 2 5	36.67
2.368	1	1 3 4	37.96
2.360	1	3 1 2	38.10
2.337	1	-3 3 3	38.49
2.330	1	2 5 0	38.60
2.329	3	-2 2 5	38.63
2.321	1	-1 5 3	38.77
2.277	2	-1 3 5	39.54
2.260	1	2 1 4	39.85
2.251	5	1 1 5	40.02
2.223	3	-1 6 1	40.55
2.185	1	-4 1 1	41.29
2.180	2	-2 3 5	41.38
2.167	1	1 2 5	41.64
2.165	1	1 5 3	41.69
2.150	1	-1 6 2	42.00
2.149	2	4 0 0	42.01
2.127	5	2 4 3	42.46
2.124	2	4 1 0	42.53
2.121	1	-4 1 3	42.60
2.113	1	0 0 6	42.76
2.108	2	-4 2 1	42.87
2.053	4	4 2 0	44.08
2.053	1	2 3 4	44.08
2.032	1	-4 0 4	44.56
2.026	2	-2 2 6	44.69
2.024	1	-3 5 1	44.75
2.021	1	0 2 6	44.80
2.015	4	4 1 1	44.96
2.013	2	-2 5 4	45.00
1.996	1	-4 3 1	45.41
1.995	1	-4 3 2	45.43
1.980	3	-3 3 5	45.78
1.949	1	4 3 0	46.57
1.942	1	1 0 6	46.74
1.932	1	2 5 3	46.98
1.930	4	1 7 0	47.04
1.925	1	-1 7 1	47.19
1.893	1	1 7 1	48.03
1.891	1	0 7 2	48.08
1.870	1	1 2 6	48.65
1.867	1	0 6 4	48.72
1.818	1	3 4 3	50.13
1.805	1	-1 2 7	50.52
1.750	1	-4 3 5	52.24
1.701	1	-5 0 4	53.86
1.700	1	-5 2 3	53.88
1.688	1	-5 1 4	54.29
1.672	1	0 8 2	54.87
1.662	1	-1 8 2	55.22
1.646	1	-1 4 7	55.82
1.622	1	-1 1 8	56.70
1.586	1	1 3 7	58.10

Phenobarbital, form III, $C_{12}H_{12}N_2O_3$

Synonyms
1. 5-Ethyl-5-phenylbarbituric acid
2. Phenobarbitone
3. Luminal
4. Phenemal
5. Phenylethylmalonylurea

CAS registry no.
50-06-6

Structure
Monoclinic, $P2_1/c$ (14), Z = 4. The structure was determined by Williams [1974].

Atom positions
All atoms are in general positions 4(e) [ibid.].

Polymorphism
There may be as many as 12 anhydrous forms of phenobarbital, as well as the monohydrate and perhaps other hydrates [ibid.].

Lattice constants
a = 9.535(2) Å
b = 11.856(3)
c = 10.795(3)
β = 111.56(1)°

(published values: a = 9.534(2) Å, b = 11.855(3), c = 10.794(3), β = 111.56(1)° [Williams, 1974])

CD cell: a = 10.795(3) Å, b = 11.856(3), c = 9.535(2), β = 111.56(1)°; sp. gp. $P2_1/a$; a/b = 0.9105; c/b = 0.8042

Volume
1135.0 Å

Density
(calculated) 1.359 g/cm^3

Thermal parameters
Isotropic for hydrogen atoms [Williams, 1974]. Isotropic B_i for other atoms, estimated from U_{ij} for each atom.

Scattering factors
C^0, H^0, N^0, O^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 1.581 \times 10^{-3}$
$I/I_{corundum}$ (calculated) 0.610 for reflection with hkℓ = $\bar{2}02$

Additional pattern
1. PDF card 5-0324 [Huang, 1951]

References

Huang, T.-Y. (1951). Acta Pharm. Int. 2, 43.
International Tables for X-ray Chrystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.
Williams, P. P. (1974). Acta Crystallogr. B30, 12.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
8.86	30	1 0 0	9.98
7.66	10	0 1 1	11.54
7.10	40	1 1 0	12.46
6.82	51	-1 1 1	12.98
5.93	2	0 2 0	14.94
5.273	40	-1 0 2	16.80
5.104	86	0 2 1	17.36
5.018	44	0 0 2	17.66
4.924	14	1 2 0	18.00
4.828	8	-1 2 1+	18.36
4.619	3	0 1 2	19.20
4.410	15	-2 1 1	20.12
4.168	100	-2 0 2	21.30
4.103	48	1 2 1	21.64
3.808	15	1 0 2	23.34
3.708	14	-2 2 1	23.98
3.625	3	1 1 2	24.54
3.551	10	2 2 0	25.06
3.440	17	2 1 1	25.88
3.245	3	1 3 1	27.46
3.198	27	-2 1 3	27.88
3.164	3	-1 3 2	28.18
3.104	40	0 3 2	28.74
3.040	2	-2 3 1	29.36
2.949	26	2 3 0	30.28
2.914	5	0 2 3	30.66
2.841	2	0 4 1	31.46
2.793	2	-3 2 1+	32.02
2.733	5	1 1 3	32.74
2.706	14	-3 1 3	33.08
2.629	4	1 4 1	34.08
2.552	3	0 4 2+	35.14
2.516	4	-3 2 3	35.66
2.510	5	0 0 4	35.74
2.465	8	2 4 0+	36.42
2.435	4	-3 3 2	36.88
2.396	6	-3 0 4	37.50
2.372	3	3 2 1	37.90
2.368	2	3 3 0	37.96
2.339	5	1 4 2	38.46
2.334	4	-4 1 2	38.54
2.308	1	2 3 2+	39.00
2.287	7	-1 4 3+	39.36
2.254	2	2 1 3	39.96
2.232	3	-4 1 3	40.38
2.218	1	0 4 3+	40.64
2.212	2	1 0 4+	40.76
2.194	2	-2 3 4	41.10
2.189	2	1 5 1+	41.20
2.174	2	1 1 4+	41.50

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.101	2	-1 1 5	43.02
2.084	1	-4 0 4	43.38
2.076	1	3 2 2+	43.56
2.061	1	-2 5 2	43.90
2.053	2	-4 1 4	44.08
2.036	2	-4 3 2	44.46
2.009	1	-1 2 5	45.10
1.980	4	2 5 1+	45.80
1.975	3	0 6 0+	45.90
1.967	3	-4 2 4	46.12
1.933	5	3 3 2+	46.98
1.898	1	-3 5 1	47.88
1.878	1	-1 3 5+	48.44
1.873	2	3 1 3	48.58
1.855	2	-5 1 3	49.06
1.846	4	-4 1 5	49.34
1.841	3	0 6 2	49.46
1.813	1	2 4 3+	50.30
1.804	1	2 6 0	50.54
1.798	2	1 1 5+	50.72
1.773	1	5 0 0+	51.50
1.754	1	1 6 2+	52.10
1.732	1	2 6 1+	52.82
1.715	1	-5 2 4+	53.38
1.685	1	-3 4 5	54.42
1.671	1	-4 5 1+	54.90
1.651	2	-5 1 5+	55.62
1.639	1	3 0 4	56.06
1.592	1	-2 5 5+	57.86
1.582	1	2 7 0+	58.28

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
8.87	28	1 0 0	9.97
7.66	9	0 1 1	11.54
7.10	36	1 1 0	12.45
6.82	47	-1 1 1	12.97
5.93	2	0 2 0	14.93
5.278	38	-1 0 2	16.78
5.129	13	1 1 1	17.27
5.105	76	0 2 1	17.36
5.020	39	0 0 2	17.65
4.928	11	1 2 0	17.98
4.831	5	-1 2 1	18.35
4.822	2	-1 1 2	18.38
4.623	2	0 1 2	19.18
4.434	1	2 0 0	20.01
4.411	14	-2 1 1	20.11
4.169	100	-2 0 2	21.29
4.105	45	1 2 1	21.63
3.809	15	1 0 2	23.33
3.708	15	-2 2 1	23.98
3.627	3	1 1 2	24.53
3.551	10	2 2 0	25.06
3.443	3	-1 1 3	25.86
3.442	15	2 1 1	25.86
3.246	3	1 3 1	27.46
3.205	5	1 2 2	27.82
3.199	25	-2 1 3	27.87
3.164	1	-1 3 2	28.19
3.105	41	0 3 2	28.73
3.092	9	-3 0 2	28.85
3.076	1	-1 2 3	29.01
3.075	5	2 2 1	29.01
3.039	1	-2 3 1	29.37
2.956	3	3 0 0	30.21
2.950	26	2 3 0	30.27
2.914	4	0 2 3	30.65
2.843	2	0 4 1	31.44
2.794	2	-3 2 1	32.00
2.741	1	-3 2 2	32.64
2.733	5	1 1 3	32.74
2.706	15	-3 1 3	33.08
2.639	1	-2 0 4	33.94
2.629	4	1 4 1	34.08
2.554	1	0 3 3	35.11
2.552	2	0 4 2	35.13
2.517	4	-3 2 3	35.65
2.510	3	0 0 4	35.75
2.472	4	-3 3 1	36.31
2.464	7	2 4 0	36.43
2.435	4	-3 3 2	36.88
2.396	6	-3 0 4	37.50
2.373	2	3 2 1	37.88
2.367	1	3 3 0	37.98
2.339	5	1 4 2	38.45
2.330	2	-4 1 2	38.61
2.288	5	-1 4 3	39.35
2.287	3	2 4 1	39.36
2.254	2	2 1 3	39.96
2.232	3	-4 1 3	40.39
2.219	1	0 4 3	40.63
2.211	1	1 0 4	40.77
2.195	2	-2 3 4	41.09
2.189	1	1 5 1	41.21
2.178	1	3 1 2	41.42
2.174	1	1 1 4	41.50
2.101	2	-1 1 5	43.02

Phenobarbital, form III, $C_{12}H_{12}N_2O_3$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.085	1	-4 0 4	43.37
2.061	1	-2 5 2	43.89
2.053	2	-4 1 4	44.07
2.036	2	-4 3 2	44.45
2.008	1	-1 2 5	45.11
1.980	3	2 5 1	45.80
1.976	1	0 6 0	45.89
1.971	1	-2 4 4	46.01
1.967	2	-4 2 4	46.12
1.933	4	3 3 2	46.97
1.930	1	1 3 4	47.05
1.898	1	-3 5 1	47.88
1.878	1	-1 3 5	48.43
1.873	2	3 1 3	48.58
1.855	2	-5 1 3	49.06
1.846	4	-4 1 5	49.33
1.839	1	0 6 2	49.54
1.805	1	2 6 0	50.53
1.799	2	1 1 5	50.72
1.732	1	2 6 1	52.82
1.684	1	-3 4 5	54.43
1.671	1	-4 5 1	54.91
1.651	2	-5 1 5	55.61
1.649	1	2 5 3	55.68

Potassium Barium Iron Titanium Oxide, $K_{1.16}Ba_{0.72}Fe_{0.36}Ti_{5.58}O_{13}$

Structure
Monoclinic, C2/m (12), Z = 2. The structure was refined using data from a natural mineral found in the Kimberley Division of Western Australia [Bagshaw et al., 1977]. Electron microprobe analysis gave the composition listed [ibid.].

Atom positions
Bagshaw et al. [1977]

2(a) 2 oxygen
4(i) 4 oxygen in each of 6 different sites
4(i) 3.72 titanium and 0.24 iron in each of 3 different sites
4(i) 2.32 potassium and 1.44 barium

Lattice constants
a = 15.454(2) Å
b = 3.8370(7)
c = 9.124(2)
β = 99.25(1)°

a/b = 4.0276
c/b = 2.3779

(published values: a = 15.453(2) Å, b = 3.8368(7), c = 9.123(2), β = 99.25(1)° [Bagshaw et al., 1977].

Volume
533.99 Å^3

Density
3.978 g/cm^3

Thermal parameters
Isotropic B_i estimated from U_{ij} for individual atoms

Scattering factors
K^+, Ba^{2+}, Fe^0, Ti^0, O^0 [Cromer and Mann, 1968]. K, Ba, Fe and Ti factors were corrected for dispersion [Cromer, 1965].

Scale factors (integrated intensities)
$\gamma = 0.1046 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 1.06 for reflection with hkℓ = 310.

References
Bagshaw, A. N., Doran, B. H., White, A. H., and Willis, A. C. (1977). Aust. J. Chem. 30, 1195.
Cromer, D. T. (1965). Acta Crystallogr. 18, 17.
Cromer, D. T. and Mann, J. B. (1968). Acta Crystallogr. A24, 321.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
9.000	7	0 0 1	9.82
7.622	54	2 0 0	11.60
6.339	41	-2 0 1	13.96
5.401	10	2 0 1	16.40
4.498	33	0 0 2	19.72
4.180	1	-2 0 2	21.24
3.811	1	4 0 0	23.32
3.729	23	-4 0 1+	23.84
3.630	7	2 0 2	24.50
3.324	5	4 0 1	26.80
3.171	14	-4 0 2	28.12
3.062	96	3 1 0	29.14
2.988	100	-3 1 1	29.88
2.959	68	-2 0 3	30.18
2.925	30	-1 1 2	30.54
2.815	82	1 1 2+	31.76
2.703	44	4 0 2	33.12
2.653	26	-3 1 2+	33.76
2.556	30	-6 0 1	35.08
2.425	2	3 1 2	37.04
2.383	11	-1 1 3+	37.72
2.349	4	6 0 1	38.28
2.251	5	0 0 4+	40.02
2.239	10	5 1 1	40.24
2.115	4	-6 0 3	42.72
2.092	52	-4 0 4	43.22
2.075	47	6 0 2	43.58
2.047	14	3 1 3	44.22
1.9952	11	-5 1 3	45.42
1.9602	7	-1 1 4	46.28
1.9187	59	0 2 0	47.34
1.8939	11	1 1 4+	48.00
1.8604	2	2 2 0	48.92
1.8378	5	-6 0 4+	49.56
1.8145	2	4 0 4	50.24
1.8038	14	7 1 1+	50.56
1.7641	7	0 2 2+	51.78
1.7515	9	-5 1 4	52.18
1.7138	7	-7 1 3	53.42
1.7067	4	-4 2 1	53.66
1.6961	2	2 2 2	54.02
1.6927	1	2 0 5	54.14
1.6649	8	7 1 2	55.12
1.6615	6	4 2 1+	55.24
1.6419	3	-4 2 2	55.96
1.6227	4	-3 1 5	56.68
1.6164	4	0 2 3	56.92
1.6097	14	-2 2 3	57.18
1.5964	5	1 1 5+	57.70
1.5859	4	-8 0 4	58.12

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.5643	16	4 2 2	59.00
1.5609	18	-7 1 4	59.14
1.5547	6	2 2 3	59.40
1.5505	7	9 1 0	59.58
1.5346	20	-6 2 1+	60.26
1.5254	5	10 0 0	60.66
1.5209	14	-10 0 2	60.86
1.5097	5	7 1 3	61.36
1.5009	10	0 0 6	61.76

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
9.005	6	0 0 1	9.81
7.627	48	2 0 0	11.59
6.345	38	-2 0 1	13.95
5.407	9	2 0 1	16.38
4.503	33	0 0 2	19.70
4.183	1	-2 0 2	21.22
3.813	1	4 0 0	23.31
3.734	20	-4 0 1	23.81
3.721	8	1 1 0	23.89
3.630	7	2 0 2	24.50
3.325	5	4 0 1	26.79
3.172	14	-4 0 2	28.11
3.063	100	3 1 0	29.13
3.002	9	0 0 3	29.74
2.989	100	-3 1 1	29.87
2.960	66	-2 0 3	30.17
2.925	28	-1 1 2	30.54
2.818	44	3 1 1	31.73
2.815	48	1 1 2	31.77
2.704	48	4 0 2	33.11
2.655	18	-3 1 2	33.73
2.652	11	2 0 3	33.77
2.556	33	-6 0 1	35.07
2.426	2	3 1 2	37.03
2.384	4	-5 1 1	37.71
2.382	8	-1 1 3	37.73
2.350	4	6 0 1	38.27
2.260	1	-2 0 4	39.85
2.256	1	-3 1 3	39.93
2.251	4	0 0 4	40.02
2.239	10	5 1 1	40.24
2.115	3	-6 0 3	42.72
2.091	58	-4 0 4	43.22
2.075	52	6 0 2	43.57
2.047	16	3 1 3	44.21

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.9950	13	-5 1 3	45.43
1.9606	7	-1 1 4	46.27
1.9292	1	-8 0 1	47.07
1.9185	69	0 2 0	47.35
1.9087	4	-7 1 1	47.60
1.9041	1	-3 1 4	47.73
1.8948	3	7 1 0	47.97
1.8936	9	1 1 4	48.01
1.8605	1	2 2 0	48.92
1.8385	4	-6 0 4	49.54
1.8364	2	-2 2 1	49.60
1.8151	1	4 0 4	50.22
1.8081	1	2 2 1	50.43
1.8073	8	8 0 1	50.45
1.8041	10	7 1 1	50.55
1.8023	2	6 0 3	50.60
1.7650	4	0 2 2	51.75
1.7637	4	5 1 3	51.79
1.7518	10	-5 1 4	52.17
1.7141	8	-7 1 3	53.41
1.7064	4	-4 2 1	53.67
1.6962	1	2 2 2	54.02
1.6930	1	2 0 5	54.13
1.6652	10	7 1 2	55.11
1.6617	1	4 2 1	55.23
1.6416	3	-4 2 2	55.97
1.6227	4	-3 1 5	56.68
1.6165	3	0 2 3	56.92
1.6099	17	-2 2 3	57.17
1.5968	5	1 1 5	57.69
1.5956	1	-6 0 5	57.73
1.5861	4	-8 0 4	58.11
1.5668	5	-9 1 1	58.90
1.5652	1	6 0 4	58.96
1.5646	14	4 2 2	58.99
1.5612	12	-7 1 4	59.13
1.5544	4	2 2 3	59.42
1.5503	5	9 1 0	59.59
1.5371	7	-9 1 2	60.15
1.5360	12	4 0 5	60.20
1.5344	13	-6 2 1	60.27
1.5337	2	-5 1 5	60.30
1.5253	3	10 0 0	60.66
1.5209	13	-10 0 2	60.86
1.5197	2	-2 0 6	60.91
1.5099	5	7 1 3	61.35
1.5009	12	0 0 6	61.76

Procaine Hydrochloride, $C_{13}H_{21}ClN_2O_2$

Synonyms
1. Novocaine hydrochloride
2. p-Aminobenzoyldiethylaminoethanol hydrochloride
3. 2-Diethylaminoethyl p-aminobenzoate hydrochloride

CAS registry no.
51-05-8

Structure
Orthorhombic, Pcab (61), Z = 8. The structure was studied by Beall, Herdklotz and Sass [1970]. The parameters used here are from the refinement by Dexter [1972].

Atom positions
All atoms were in the general positions 8(c) [Dexter, 1972].

Lattice constants
a = 25.019(1) Å
b = 8.3060(5)
c = 14.193(1)

(published values: a = 25.017(1) Å, b = 8.3050(5), c = 14.192(1) [Dexter, 1972])

CD cell: a = 14.193(1) Å, b = 25.019(1), c = 8.3060(5); sp. gp. Pcab; a/b = 0.5673; c/b = 0.3320

Volume
2949.4 $Å^3$

Density
(calculated) 1.229 g/cm^3

Thermal parameters
Isotropic: hydrogen atoms, overall B = 4.0 [Dexter, 1972].
Isotropic B_i for other atoms, estimated from U_{ij} for each atom.

Scattering factors
C^0, H^0, N^0, O^0, Cl^- [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.5173 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 0.601, for reflection with hkℓ = 113.

Additional patterns
1. PDF card 27-1975 [Wang, P. Polytechnic Inst. of New York, 1975]
2. Folen [1975]

References
Beall, E., Herdklotz, J., and Sass, R. L. (1970). Biochem. Biophys. Res. Commun. 39, 329.
Dexter, D. D. (1972). Acta Crystallogr. B28, 77.
Folen, V. A. (1975). J. Forensic Sci. 20, 348.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2Θ(°) λ - 1.540598Å
12.51	7	2 0 0	7.06
7.09	6	0 0 2	12.48
6.89	35	1 1 1	12.84
6.22	37	2 1 1+	14.22
5.434	79	3 1 1	16.30
5.401	66	0 1 2	16.40
4.951	4	2 1 2	17.90
4.692	7	4 0 2	18.90
4.423	16	2 0 3	20.06
4.153	59	0 2 0	21.38
4.100	33	5 1 1	21.66
4.055	100	1 1 3	21.90
3.9039	28	2 1 3	22.76
3.7954	2	2 2 1	23.42
3.7171	18	3 2 0	23.92
3.6688	16	5 1 2	24.24
3.6015	9	6 1 1	24.70
3.5478	24	0 0 4	25.08
3.4347	6	4 1 3	25.92
3.4140	4	2 0 4	26.08
3.3608	3	4 2 1	26.50
3.2925	4	6 1 2+	27.06
3.2618	15	0 1 4	27.32
3.2362	8	1 1 4	27.54
3.1975	17	7 1 1	27.88
3.1752	31	5 1 3	28.08
3.1272	15	6 0 3+	28.52
3.0953	22	1 2 3	28.82
3.0275	3	2 2 3	29.48
2.9781	2	7 1 2	29.98
2.9229	9	3 2 3+	30.56
2.8662	5	8 1 1	31.18
2.7929	2	4 2 3	32.02
2.7677	1	2 0 5	32.32
2.7170	3	6 2 2	32.94
2.6979	12	0 2 4+	33.18
2.6483	10	5 2 3	33.82
2.6079	3	8 0 3	34.36
2.5788	15	0 3 2+	34.76
2.5253	6	2 3 2	35.52
2.4927	6	4 3 1+	36.00
2.4702	3	9 1 2	36.34
2.4650	3	10 0 1	36.42
2.3781	2	1 3 3	37.80
2.3612	4	5 1 5+	38.08

d(Å)	I	hkℓ			2θ(°) λ - 1.540598Å
2.3470	6	2	3	3+	38.32
2.3019	2	9	1	3+	39.10
2.2929	3	5	3	2	39.26
2.2762	5	6	3	1+	39.56
2.2652	5	1	1	6+	39.76
2.2587	5	6	1	5	39.88
2.2109	1	10	0	3	40.78
2.1934	2	6	3	2+	41.12
2.1822	3	0	3	4	41.34
2.1436	2	7	1	5+	42.12
2.0907	1	7	3	2	43.24
2.0851	2	12	0	0	43.36
2.0769	2	0	4	0	43.54
2.0439	4	10	0	4+	44.28
2.0283	1	2	2	6+	44.64
1.9952	3	11	2	0+	45.42
1.9903	3	11	1	3+	45.54
1.9594	2	7	2	5	46.30
1.9318	1	9	1	5+	47.00
1.9179	1	5	4	0+	47.36
1.8991	2	8	3	3+	47.86
1.8582	1	13	1	1+	48.98
1.8540	1	3	4	3	49.10
1.8385	2	10	3	1+	49.54
1.8344	2	5	1	7+	49.66
1.8166	1	1	2	7	50.18
1.8125	2	13	1	2	50.30
1.7978	3	0	3	6+	50.74
1.7899	4	6	3	5+	50.98
1.7814	3	7	4	1+	51.24
1.7776	2	5	4	3+	51.36
1.7566	1	2	0	8+	52.02
1.7429	2	13	1	3+	52.46
1.7300	2	1	1	8+	52.88
1.7120	2	5	2	7+	53.48
1.7073	2	4	0	8	53.64
1.6392	2	5	1	8+	56.06
1.6280	1	1	2	8	56.48
1.6222	2	2	3	7+	56.70
1.6180	1	3	5	1+	56.86
1.6040	1	2	5	2+	57.40
1.5667	2	5	5	1+	58.90
1.5600	1	0	4	6+	59.18
1.5547	1	10	3	5+	59.40

Calculated Pattern (Integrated)					
d(Å)	I	hkℓ			2θ(°) λ - 1.540598Å
12.51	7	2	0	0	7.06
7.10	5	0	0	2	12.46
6.89	33	1	1	1	12.84
6.25	22	4	0	0	14.15
6.22	23	2	1	1	14.23
6.17	5	2	0	2	14.34
5.436	67	3	1	1	16.29
5.395	48	0	1	2	16.42
4.954	4	2	1	2	17.89
4.713	1	4	1	1	18.81
4.692	7	4	0	2	18.90
4.425	15	2	0	3	20.05
4.153	58	0	2	0	21.38
4.103	21	5	1	1	21.64
4.097	2	1	2	0	21.67
4.085	1	4	1	2	21.74
4.057	100	1	1	3	21.89
4.001	4	6	0	1	22.20
3.9415	1	2	2	0	22.54
3.9362	1	1	2	1	22.57
3.9054	28	2	1	3	22.75
3.7977	1	2	2	1	23.41
3.7176	17	3	2	0	23.92
3.6873	9	3	1	3	24.12
3.6689	13	5	1	2	24.24
3.6044	8	6	1	1	24.68
3.5843	2	0	2	2	24.82
3.5482	25	0	0	4	25.08
3.4353	5	4	1	3	25.91
3.4136	3	2	0	4	26.08
3.3614	3	4	2	1	26.50
3.2993	2	6	1	2	27.00
3.2931	1	3	2	2	27.06
3.2630	15	0	1	4	27.31
3.2356	7	1	1	4	27.55
3.1986	14	7	1	1	27.87
3.1764	31	5	1	3	28.07
3.1573	2	2	1	4	28.24
3.1282	8	6	0	3	28.51
3.1274	6	8	0	0	28.52
3.1177	1	5	2	1	28.61
3.0971	22	1	2	3	28.80
3.0862	2	4	0	4	28.91
3.0282	2	2	2	3	29.47
2.9797	2	7	1	2	29.96
2.9425	1	6	2	0	30.35
2.9231	9	3	2	3	30.56
2.9139	3	5	2	2	30.66
2.8665	5	8	1	1	31.18
2.7927	2	4	2	3	32.02

Procaine Hydrochloride, $C_{13}H_{21}ClN_2O_2$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.7682	1	2 0 5	32.31
2.7181	2	6 2 2	32.93
2.7016	1	1 3 1	33.13
2.6977	9	0 2 4	33.18
2.6973	3	7 1 3	33.19
2.6822	4	1 2 4	33.38
2.6610	4	7 2 1	33.65
2.6482	10	5 2 3	33.82
2.6371	1	2 2 4	33.97
2.6089	2	8 0 3	34.35
2.5849	5	4 0 5	34.68
2.5793	13	0 3 2	34.75
2.5668	4	3 2 4	34.93
2.5567	3	3 1 5	35.07
2.5309	1	7 2 2	35.44
2.5262	5	2 3 2	35.51
2.5019	4	10 0 0	35.86
2.4987	1	6 2 3	35.91
2.4924	4	4 3 1	36.01
2.4712	2	9 1 2	36.33
2.4639	1	10 0 1	36.44
2.3880	1	5 3 1	37.64
2.3787	2	1 3 3	37.79
2.3666	2	5 1 5	37.99
2.3622	2	10 1 1	38.06
2.3471	4	2 3 3	38.32
2.3465	2	6 0 5	38.33
2.3028	1	9 1 3	39.08
2.2926	2	5 3 2	39.27
2.2801	1	9 2 1	39.49
2.2767	4	6 3 1	39.55
2.2750	1	0 1 6	39.58
2.2657	3	1 1 6	39.75
2.2650	1	6 2 4	39.76
2.2581	3	6 1 5	39.89
2.2117	1	10 0 3	40.77
2.1936	1	6 3 2	41.12
2.1828	3	0 3 4	41.33
2.1473	1	7 1 5	42.04
2.1431	1	10 2 0	42.13
2.0916	1	7 3 2	43.22
2.0849	1	12 0 0	43.36
2.0765	2	0 4 0	43.55
2.0486	1	1 2 6	44.17
2.0447	3	10 0 4	44.26
2.0430	1	6 2 5	44.30
1.9971	1	6 1 6	45.37
1.9949	2	11 2 0	45.43
1.9902	2	11 1 3	45.54
1.9598	2	7 2 5	46.29
1.9317	1	9 1 5	47.00
1.9179	1	5 4 0	47.36
1.8987	2	8 3 3	47.87
1.8587	1	13 1 1	48.97
1.8538	1	3 4 3	49.10
1.8430	1	6 4 1	49.41
1.8406	1	10 3 1	49.48
1.8381	1	11 2 3	49.55
1.8172	1	1 2 7	50.16
1.8127	2	13 1 2	50.30
1.7985	2	0 3 6	50.72
1.7901	3	6 3 5	50.98
1.7876	1	1 4 4	51.05
1.7813	1	7 4 1	51.25
1.7774	1	5 4 3	51.36
1.7462	1	13 2 0	52.35
1.7430	2	13 1 3	52.46
1.7308	1	1 1 8	52.85
1.7121	2	5 2 7	53.48
1.7068	1	4 0 8	53.66
1.6392	1	5 1 8	56.06
1.6323	1	1 3 7	56.32
1.6280	1	1 2 8	56.48
1.6220	1	2 3 7	56.71
1.6041	1	2 5 2	57.40
1.5670	1	5 5 1	58.89
1.5667	1	13 2 4	58.90

Psilocin, $C_{12}H_{16}N_2O$

Synonyms
1. 3-(2-(Dimethylamino)ethyl)-indol-4-ol
2. 4-Hydroxy-N,N-dimethyltryptamine

CAS registry no.
520-53-6

Structure
Monoclinic, $P2_1/c$ (14), Z = 4. The structure was determined by Petcher and Weber [1974].

Atom positions
All the atoms were in general positions 4(e). For H(7), the value 0.273 was used for "z" as given in the Supplementary Publ. #SUP20980, referred to by Petcher and Weber [1974]. Bond length calculations indicated that the value of 0.014 for "z" for H(12) should be used.

Lattice constants
a = 10.60(3) Å
b = 8.53(2)
c = 12.51(3)
β = 91.25(30)°
[Petcher and Weber, 1974]

CD cell: a = 12.51(3) Å, b = 8.53(2), c = 10.60(3), β = 91.25(30)°; sp. gp. $P2_1/a$; a/b = 1.4665, c/b = 1.2426

Volume
1131. $Å^3$

Density
(calculated) 1.200 g/cm^3
(measured) 1.19 [Petcher and Weber, 1974]

Thermal parameters
Isotropic B_i estimated from β_{ij} for individual atoms.

Scattering factors
Zero ionization [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 3.259 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 1.06 for reflection with hkℓ = 112.

Additional pattern
1. PDF card 13-981 [Physical Data of Indole and Dihydroindole Alkaloids, edited by Neuss, Eli Lilly and Co., 1962]

References

International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.
Petcher, T. J. and Weber, H. P. (1974). J. Chem. Soc. Perkin Trans. 2, 946.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
10.59	51	1 0 0	8.34
7.04	10	0 1 1	12.56
6.64	6	1 1 0	13.32
6.25	1	0 0 2	14.16
5.89	5	-1 1 1	15.02
5.83	9	1 1 1	15.18
5.43	2	-1 0 2	16.30
5.30	22	2 0 0	16.72
5.04	12	0 1 2	17.58
4.58	33	-1 1 2	19.36
4.52	100	1 1 2	19.62
4.26	22	0 2 0	20.82
4.21	21	2 1 1	21.10
4.08	4	-2 0 2	21.74
4.00	3	2 0 2	22.22
3.96	6	1 2 0	22.46
3.76	47	1 2 1	23.64
3.62	2	2 1 2	24.56
3.51	2	1 1 3	25.36
3.33	9	1 2 2	26.74
3.26	1	3 1 0	27.32
3.20	5	2 2 1	27.86
3.09	1	-2 1 3	28.90
3.05	2	3 0 2	29.30
2.934	4	0 1 4	30.44
2.917	6	2 2 2	30.62
2.857	5	1 2 3	31.28
2.773	5	0 3 1	32.26
2.746	2	1 3 0	32.58
2.648	1	3 2 1	33.82
2.615	2	-2 2 3	34.26
2.509	6	1 3 2+	35.76
2.479	1	3 2 2	36.20
2.461	2	-2 3 1+	36.48
2.443	2	1 2 4	36.76
2.367	1	-3 0 4	37.98
2.317	1	2 3 2+	38.84
2.281	1	-3 1 4	39.48
2.261	2	2 2 4	39.84
2.207	1	4 2 1	40.86
2.138	1	2 3 3	42.24
2.120	2	5 0 0	42.62
2.079	1	3 3 2	43.50
2.043	1	-4 0 4	44.30
2.018	1	0 4 2	44.88
1.995	2	-4 2 3+	45.42
1.955	1	-2 0 6	46.42
1.945	1	3 3 3	46.66
1.796	1	3 3 4+	50.80
1.669	1	-3 3 5+	54.96
1.665	1	2 4 4	55.10

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
10.60	47	1 0 0	8.34
7.05	10	0 1 1	12.55
6.64	5	1 1 0	13.31
6.25	1	0 0 2	14.15
5.90	4	-1 1 1	15.00
5.84	8	1 1 1	15.17
5.44	1	-1 0 2	16.29
5.34	1	1 0 2	16.60
5.30	21	2 0 0	16.72
5.04	12	0 1 2	17.57
4.59	28	-1 1 2	19.34
4.52	100	1 1 2	19.61
4.50	1	2 1 0	19.71
4.26	18	0 2 0	20.81
4.26	3	-2 1 1	20.83
4.21	20	2 1 1	21.08
4.09	3	-2 0 2	21.73
4.00	3	2 0 2	22.21
3.96	6	1 2 0	22.45
3.76	51	1 2 1	23.62
3.75	1	0 1 3	23.74
3.62	2	2 1 2	24.56
3.51	2	1 1 3	25.35
3.36	2	-1 2 2	26.54
3.33	10	1 2 2	26.74
3.26	1	3 1 0	27.30
3.20	5	2 2 1	27.86
3.09	1	-2 1 3	28.90
3.05	2	3 0 2	29.28
3.03	1	2 1 3	29.45
2.936	4	0 1 4	30.42
2.918	6	2 2 2	30.62
2.858	6	1 2 3	31.27
2.773	5	0 3 1	32.26
2.746	2	1 3 0	32.58
2.649	1	3 2 1	33.81
2.616	2	-2 2 3	34.25
2.510	1	-3 2 2	35.74
2.509	6	1 3 2	35.76
2.479	1	3 2 2	36.20
2.462	2	-2 3 1	36.47
2.444	2	1 2 4	36.75
2.367	1	-3 0 4	37.98
2.317	1	2 3 2	38.83
2.281	1	-3 1 4	39.48
2.262	3	2 2 4	39.83
2.208	1	4 2 1	40.84
2.138	1	2 3 3	42.24
2.119	2	5 0 0	42.62
2.079	1	3 3 2	43.50
2.043	1	-4 0 4	44.29
1.996	1	-4 2 3	45.40
1.994	1	5 0 2	45.45
1.954	1	-2 0 6	46.42
1.945	1	3 3 3	46.66
1.796	1	3 3 4	50.80
1.782	1	2 4 3	51.23
1.666	1	2 4 4	55.09

Psilocybin Methanolate, $C_{13}H_{21}N_2O_4P$

Synonyms
1. Indocybin
2. 3-[2-(Dimethylamino)ethyl]indol-4-ol dihydrogen phosphate methanolate

CAS registry no.
520-52-5

Structure
Monoclinic, $P2_1/c$ (14), Z = 8. The structure was determined by Weber and Petcher [1974].

Atom positions
All atoms were in general positions 4(e).

Lattice constants
a = 12.64(1) Å
b = 29.11(2)
c = 8.848(6)
β = 107.37(2)°

a/b = 0.4342
c/b = 0.3040

(published values: a = 12.64(1) Å, b = 29.11(2), c = 8.847(6), β = 107.37(2)° [Weber and Petcher, 1974])

Volume
3107. Å^3

Density
(calculated) 1.352 g/cm^3
(measured) 1.34 [Weber and Petcher, 1974]

Thermal parameters
Isotropic, for hydrogens [Weber and Petcher, 1974]. For all other atoms, B_i were estimated for β_{ij} for individual atoms.

Scattering factors
Zero ionization [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 0.5540 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 0.455 for reflection with hkℓ = 120.

Additional patterns
1. PDF card 13-982 [Physical Data of Indole and Dihydroindole Alkaloids edited by Neuss, Eli Lilly and Co., 1962]
2. Folen [1975]

References

Folen, V. A. (1975). J. Forensic Sci. 20, 348.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.
Weber, H. P. and Petcher, T. J. (1974). J. Chem. Soc. Perkin Trans. 2, p. 942.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
14.52	1	0 2 0	6.08
12.07	2	1 0 0	7.32
11.13	2	1 1 0	7.94
9.28	100	1 2 0	9.52
8.11	24	0 1 1	10.90
7.56	4	1 3 0	11.70
7.27	41	0 4 0+	12.16
7.11	74	-1 2 1	12.44
6.23	5	-1 3 1+	14.20
5.98	38	1 1 1	14.80
5.63	14	1 2 1	15.72
5.51	50	0 4 1	16.08
5.43	14	-1 4 1	16.32
5.24	16	1 5 0	16.90
5.17	15	1 3 1	17.14
4.97	8	-2 3 1	17.82
4.79	3	0 5 1	18.50
4.74	2	-1 5 1	18.72
4.68	3	1 4 1	18.96
4.64	2	2 4 0	19.10
4.50	49	1 6 0	19.72
4.367	30	-1 1 2	20.32
4.283	7	2 1 1	20.72
4.219	35	0 0 2+	21.04
4.172	42	-1 6 1+	21.28
4.096	17	-3 1 1	21.68
4.041	46	-2 1 2+	21.98
3.983	18	-3 2 1+	22.30
3.955	15	2 3 1	22.46
3.928	19	1 7 0+	22.62
3.870	16	0 3 2	22.96
3.779	32	2 6 0+	23.52
3.708	18	-1 7 1+	23.98
3.657	30	1 0 2	24.32
3.599	11	-3 4 1	24.72
3.556	50	-2 4 2	25.02
3.450	11	-3 1 2	25.80
3.424	10	2 7 0+	26.00
3.376	5	-2 7 1+	26.38
3.339	6	0 8 1+	26.68
3.309	4	3 5 0	26.92
3.266	37	1 4 2+	27.28
3.184	2	0 6 2	28.00
3.149	3	-3 6 1	28.32
3.125	4	1 8 1+	28.54
3.097	12	1 5 2	28.80
3.019	9	0 9 1+	29.56
3.000	8	4 1 0+	29.76
2.953	8	4 2 0	30.24
2.921	2	1 6 2+	30.58

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.895	6	-4 0 2	30.86
2.882	6	-4 1 2+	31.00
2.852	4	1 9 1+	31.34
2.819	4	2 4 2+	31.72
2.776	3	-4 3 2+	32.22
2.741	5	-1 10 1	32.64
2.698	3	-2 4 3+	33.18
2.667	2	-3 7 2	33.58
2.618	3	-3 3 3	34.22
2.611	3	-1 9 2	34.32
2.592	4	2 9 1+	34.58
2.564	4	4 2 1+	34.96
2.548	3	-3 9 1+	35.20
2.535	3	0 5 3+	35.38
2.513	4	-4 7 1+	35.70
2.490	2	1 3 3+	36.04
2.462	2	-3 5 3	36.46
2.445	3	-4 1 3+	36.72
2.434	5	0 6 3	36.90
2.413	3	5 0 0+	37.24
2.398	2	-5 2 2+	37.48
2.378	3	4 5 1+	37.80
2.372	3	-2 10 2+	37.90
2.341	2	5 3 0+	38.42
2.327	1	-4 4 3	38.66
2.319	2	-5 5 1	38.80
2.290	4	5 4 0+	39.32
2.270	2	-2 8 3+	39.68
2.202	2	1 13 0+	40.96
2.193	4	2 4 3+	41.12
2.189	4	1 7 3+	41.20
2.173	2	-5 6 2+	41.52
2.160	2	-5 7 1+	41.78
2.140	3	2 5 3+	42.20
2.126	1	-1 12 2+	42.48
2.118	1	4 8 1+	42.66
2.103	1	1 13 1+	42.98

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
14.55	1	0 2 0	6.07
12.06	2	1 0 0	7.32
11.14	2	1 1 0	7.93
9.29	100	1 2 0	9.51
8.11	24	0 1 1	10.90
7.56	3	1 3 0	11.69
7.30	10	0 2 1	12.11
7.28	31	0 4 0	12.15
7.11	74	-1 2 1	12.43
6.24	3	-1 3 1	14.17
6.23	2	1 4 0	14.20
6.03	1	2 0 0	14.67
5.98	39	1 1 1	14.79
5.68	5	-2 1 1	15.58
5.64	12	1 2 1	15.71
5.51	52	0 4 1	16.06
5.43	11	-1 4 1	16.31
5.24	16	1 5 0	16.90
5.17	15	1 3 1	17.13
5.12	1	2 3 0	17.30
4.97	8	-2 3 1	17.82
4.79	3	0 5 1	18.50
4.74	1	-1 5 1	18.71
4.68	2	1 4 1	18.94
4.64	1	2 4 0	19.10
4.53	12	-2 4 1	19.57
4.50	51	1 6 0	19.71
4.368	32	-1 1 2	20.32
4.287	5	2 1 1	20.70
4.227	11	-1 2 2	21.00
4.222	23	0 0 2	21.02
4.189	16	2 5 0	21.19
4.179	14	0 1 2	21.25
4.170	23	-1 6 1	21.29
4.154	3	2 2 1	21.37
4.107	3	-2 5 1	21.62
4.101	10	-3 1 1	21.65
4.078	8	-2 0 2	21.78
4.055	26	0 2 2	21.90
4.038	31	-2 1 2	21.99
4.021	16	3 0 0	22.09
4.021	4	-1 3 2	22.09
3.984	8	-3 2 1	22.30
3.983	5	3 1 0	22.30
3.957	10	2 3 1	22.45
3.932	11	1 7 0	22.60
3.927	7	-2 2 2	22.63
3.872	16	0 3 2	22.95
3.810	4	-3 3 1	23.33
3.800	9	1 6 1	23.39
3.780	24	2 6 0	23.51
3.776	9	-1 4 2	23.54
3.731	5	0 7 1	23.83
3.724	2	2 4 1	23.88
3.715	8	3 3 0	23.94
3.705	10	-1 7 1	24.00
3.659	33	1 0 2	24.31
3.631	2	1 1 2	24.50
3.600	8	-3 4 1	24.71
3.557	57	-2 4 2	25.01

Psilocybin Methanolate, $C_{13}H_{21}N_2O_4P$ - (continued)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
3.520	1	3 4 0	25.28
3.519	2	-1 5 2	25.29
3.476	1	-3 0 2	25.61
3.451	11	-3 1 2	25.79
3.438	2	1 7 1	25.89
3.424	3	1 3 2	26.00
3.424	5	2 7 0	26.00
3.418	1	0 5 2	26.05
3.381	1	-3 2 2	26.34
3.378	2	-2 7 1	26.36
3.375	2	-3 5 1	26.39
3.342	3	0 8 1	26.65
3.340	3	-2 5 2	26.67
3.323	2	-1 8 1	26.81
3.309	2	3 5 0	26.93
3.272	1	-3 3 2	27.23
3.269	32	1 4 2	27.26
3.266	10	-1 6 2	27.28
3.251	7	3 1 1	27.41
3.232	2	2 6 1	27.57
3.185	1	0 6 2	27.99
3.150	2	-3 6 1	28.31
3.127	3	1 8 1	28.52
3.098	13	1 5 2	28.79
3.083	3	-4 2 1	28.94
3.081	5	-2 8 1	28.95
3.028	4	-1 7 2	29.48
3.020	7	0 9 1	29.55
3.000	6	4 1 0	29.76
3.000	2	-4 3 1	29.76
2.963	1	0 7 2	30.14
2.953	9	4 2 0	30.24
2.897	5	-4 0 2	30.84
2.883	3	-4 1 2	31.00
2.880	2	4 3 0	31.03
2.859	2	1 9 1	31.26
2.852	2	3 5 1	31.34
2.848	1	-2 2 3	31.38
2.824	2	-2 9 1	31.66
2.818	2	2 4 2	31.72
2.783	1	-2 3 3	32.14
2.776	1	-4 3 2	32.22
2.742	5	-1 10 1	32.64
2.728	1	-1 4 3	32.80
2.698	2	-2 4 3	33.18
2.667	3	-3 7 2	33.58
2.628	1	1 10 1	34.09
2.618	2	-3 3 3	34.23
2.610	2	-1 9 2	34.34
2.599	1	-2 5 3	34.48

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.592	3	2 9 1	34.57
2.566	2	1 1 3	34.94
2.564	3	4 2 1	34.97
2.549	1	-3 9 1	35.17
2.547	1	-3 4 3	35.21
2.537	1	1 2 3	35.35
2.534	1	0 5 3	35.39
2.516	1	-1 6 3	35.66
2.513	1	-3 8 2	35.69
2.513	2	-4 7 1	35.70
2.490	2	1 3 3	36.04
2.463	1	-3 5 3	36.45
2.447	2	-4 1 3	36.70
2.446	1	-5 3 1	36.71
2.435	5	0 6 3	36.89
2.426	1	0 12 0	37.03
2.423	1	1 9 2	37.07
2.413	1	5 0 0	37.24
2.411	1	3 4 2	37.26
2.388	1	-5 4 1	37.64
2.382	1	-3 10 1	37.74
2.377	2	4 5 1	37.81
2.369	1	-2 10 2	37.95
2.341	2	5 3 0	38.41
2.327	1	-4 4 3	38.67
2.319	1	-5 5 1	38.81
2.295	2	4 6 1	39.23
2.290	3	5 4 0	39.31
2.278	1	1 10 2	39.53
2.270	1	-2 8 3	39.67
2.266	1	-4 8 2	39.74
2.202	1	1 13 0	40.96
2.194	2	2 4 3	41.11
2.194	2	-1 0 4	41.11
2.190	1	1 7 3	41.19
2.184	1	-2 2 4	41.31
2.173	1	-5 6 2	41.52
2.160	1	-5 7 1	41.78
2.140	2	2 5 3	42.20
2.126	1	-1 12 2	42.48
2.103	1	1 13 1	42.98

Sodium Barbital, $C_8H_{11}N_2NaO_3$

Synonyms
1. Sodium 5,5-diethylbarbiturate
2. Soluble barbital
3. Barbitone sodium
4. Sodium malonylurea

CAS registry no.
144-02-5

Structure
Orthorhombic, $P2_12_12_1$ (19), Z = 4. The structure was determined by Berking and Craven [1971]. It is isostructural with potassium barbital [Berthou et al., 1962].

Atom positions
All atoms were in general positions 4(a) [ibid.].

Lattice constants
a = 6.724(1) Å
b = 11.951(2)
c = 12.130(2)

(published values: a = 6.724(1) Å, b = 11.950(2), c = 12.129(2) [Berking and Craven, 1971])

CD cell: a = 11.951(2) Å, b = 12.130(2), c = 6.724(1); sp. gp. $P2_12_12_1$; a/b = 0.9852, c/b = 0.5543

Volume
974.75 $Å^3$

Density
(calculated) 1.405 g/cm^3
(measured) 1.408 g/cm^3 [Berking and Craven, 1971]

Thermal parameters
Isotropic for hydrogen atoms, anisotropic for non-hydrogen atoms [Berking and Craven, 1971]

Scattering factors
C^0, H^0, Na^0, N^0, O^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 1.519 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 0.877 for reflection with hkℓ = 011

Additional pattern
1. PDF card 9-512 [Parkes, E. B., South-Western Forensic Science Lab., Westbury on Trym, Bristol 9, Eng.]

References

Berking, B. and Craven, B. M. (1971). Acta Crystallogr. B27, 1107.
Berthou, J., Cavelier, C., Marek, D., Rérat, B., and Rérat, C. (1962). C. R. Acad. Sci. 255, 1632.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
8.50	100	0 1 1	10.40
6.06	26	0 0 2	14.60
5.97	17	0 2 0	14.82
5.85	65	1 1 0	15.12
5.36	53	0 2 1	16.54
5.28	8	1 1 1	16.78
4.503	6	1 0 2	19.70
4.255	51	0 2 2	20.86
4.211	30	1 1 2+	21.08
3.783	9	0 3 1	23.50
3.596	4	1 2 2	24.74
3.464	4	1 0 3	25.70
3.427	2	1 3 0	25.98
3.329	30	0 3 2+	26.76
3.236	4	2 1 0+	27.54
3.127	27	2 1 1	28.52
3.032	1	0 0 4	29.44
2.986	9	0 4 0+	29.90
2.930	3	2 2 0	30.48
2.901	3	0 4 1	30.80
2.838	16	0 3 3	31.50
2.764	1	1 0 4	32.36
2.693	3	1 1 4	33.24
2.664	6	1 4 1	33.62
2.638	4	2 2 2	33.96
2.614	8	1 3 3	34.28
2.509	5	1 2 4	35.76
2.490	2	1 4 2	36.04
2.403	7	0 4 3	37.40
2.3720	3	2 2 3+	37.90
2.3446	2	0 5 1	38.36
2.2707	5	1 3 4	39.66
2.2663	4	1 4 3	39.74
2.2522	2	1 5 0+	40.00
2.2415	4	1 1 5	40.20
2.2234	1	0 5 2	40.54
2.2140	3	1 5 1+	40.72
2.2026	7	3 1 0+	40.94
2.1672	4	3 1 1+	41.64
2.1074	2	2 2 4+	42.88
2.0679	5	3 2 1	43.74
2.0581	3	0 5 3	43.96
2.0291	5	1 4 4	44.62
1.9804	3	1 3 5	45.78
1.9602	1	2 3 4+	46.28
1.9538	2	3 3 0	46.44
1.9349	2	3 1 3+	46.92
1.8924	2	0 6 2	48.04
1.8865	3	1 6 1	48.20
1.8777	2	0 5 4	48.44

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.8683	2	2 2 5	48.7′
1.8589	3	3 3 2	48.96
1.8420	2	1 2 6	49.44
1.7985	2	2 4 4	50.72
1.7737	1	3 4 1	51.48
1.7584	1	3 3 3	51.96
1.7547	2	2 5 3	52.08
1.7410	1	1 3 6	52.52
1.7324	1	2 0 6	52.80
1.7270	1	1 6 3+	52.98
1.7191	1	3 4 2	53.24
1.7150	2	2 1 6+	53.38
1.6615	1	1 1 7+	55.24
1.6489	2	2 6 2	55.70
1.6392	3	3 4 3+	56.06
1.6159	1	1 6 4+	56.94
1.6040	1	4 2 1+	57.40
1.5784	1	3 5 2+	58.42
1.5730	1	0 7 3	58.64

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
8.51	100	0 1 1	10.38
6.06	25	0 0 2	14.59
5.98	12	0 2 0	14.81
5.88	8	1 0 1	15.05
5.86	61	1 1 0	15.11
5.36	55	0 2 1	16.52
5.28	5	1 1 1	16.79
4.504	6	1 0 2	19.70
4.257	53	0 2 2	20.85
4.214	24	1 1 2	21.06
4.191	17	1 2 1	21.18
3.785	10	0 3 1	23.49
3.597	4	1 2 2	24.73
3.465	5	1 0 3	25.69
3.427	1	1 3 0	25.98
3.362	1	2 0 0	26.49
3.349	12	0 2 3	26.60
3.330	20	0 3 2	26.75
3.328	12	1 1 3	26.77
3.298	1	1 3 1	27.01
3.240	2	2 0 1	27.51
3.236	2	2 1 0	27.54
3.127	32	2 1 1	28.52
3.032	1	0 0 4	29.43
2.998	5	1 2 3	29.78
2.988	5	0 4 0	29.88
2.984	4	1 3 2	29.92
2.930	3	2 2 0	30.48
2.901	3	0 4 1	30.80
2.855	1	2 1 2	31.30
2.848	2	2 2 1	31.38
2.838	18	0 3 3	31.50
2.764	1	1 0 4	32.36
2.693	3	1 1 4	33.24
2.664	7	1 4 1	33.62
2.638	4	2 2 2	33.95
2.614	9	1 3 3	34.27
2.509	6	1 2 4	35.76
2.490	2	1 4 2	36.05
2.403	8	0 4 3	37.39
2.3775	2	0 1 5	37.81
2.3726	2	2 2 3	37.89
2.3658	1	2 3 2	38.00
2.3451	2	0 5 1	38.35
2.2711	6	1 3 4	39.65
2.2628	1	1 4 3	39.81
2.2521	1	1 5 0	40.00
2.2415	4	1 1 5	40.20
2.2237	1	0 5 2	40.53
2.2143	2	1 5 1	40.71
2.2040	2	3 0 1	40.91
2.2029	7	3 1 0	40.93
2.1685	2	2 3 3	41.61
2.1675	3	3 1 1	41.63
2.1113	1	1 5 2	42.80
2.1072	2	2 2 4	42.88
2.0720	1	0 3 5	43.65
2.0678	6	3 2 1	43.74
2.0576	2	0 5 3	43.97
2.0291	6	1 4 4	44.62
1.9801	4	1 3 5	45.79
1.9603	1	2 3 4	46.28
1.9534	2	3 3 0	46.45
1.9361	1	1 0 6	46.89
1.9344	2	3 1 3	46.93
1.8924	2	0 6 2	48.04
1.8866	3	1 6 1	48.20
1.8772	1	0 5 4	48.45
1.8686	2	2 2 5	48.69
1.8593	3	3 3 2	48.95
1.8418	3	1 2 6	49.45
1.7983	3	2 4 4	50.73
1.7736	1	3 4 1	51.48
1.7589	1	3 3 3	51.95
1.7550	2	2 5 3	52.07

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
1.7413	1	1 3 6	52.51
1.7325	1	2 0 6	52.80
1.7194	1	3 4 2	53.23
1.7146	2	2 1 6	53.39
1.6780	1	1 0 7	54.65
1.6617	1	1 1 7	55.23
1.6491	2	2 6 2	55.69
1.6390	1	2 5 4	56.07
1.6390	2	3 4 3	56.07
1.5728	1	0 7 3	58.65

Δ^9-Tetrahydrocannabinolic Acid B, $C_{22}H_{30}O_4$

Synonyms
1. delta (sup 9) - THC acid B
2. 6,6,9-trimethyl-3-pentyl-7,8,9,10-tetrahydro-6H-dibenzo(b,d)pyran-1-ol

Structure
Orthorhombic, $P2_12_12_1$ (19), Z = 4. The structure was refined by Rosenqvist and Ottersen [1975].

Atom positions
All atoms were in general positions 4(a).

Lattice constants
a = 16.515(2) Å
b = 14.325(2)
c = 8.744(1)

(published values: a = 16.514(2) Å, b = 14.324(2), c = 8.744(1) [Rosenqvist and Ottersen, 1975])

CD cell: a = 14.325(2) Å, b = 16.514(2), c = 8.744(1). sp. gp. $P2_12_12_1$; a/b = 0.8674; c/b = 0.5295.

Volume
2068.6 $Å^3$

Density
(calculated) 1.151 g/cm^3
(measured) 1.12 g/cm^3 [Rosenqvist and Ottersen, 1975]

Thermal parameters
For hydrogen: isotropic B_i [Rosenqvist and Ottersen, 1975]
For other atoms, isotropic B_i estimated from β_{ij} for individual atoms.

Scattering factors
H^0 [Stewart et al., 1965]
C^0, O^0 [Doyle and Turner, 1968]

Scale factors (integrated intensities)
$\gamma = 3.492 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 1.20 for reflection with hkℓ = 110.

References

Doyle, P. A. and Turner, P. S. (1968). Acta Crystallogr. A24, 390.
Rosenqvist, E. and Ottersen, T. (1975). Acta Chem. Scand. B29, 379.
Stewart, R. F., Davidson, E. R., and Simpson, W. T. (1965). J. Chem. Phys. 42, 3175.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
10.80	100	1 1 0	8.18
8.25	6	2 0 0	10.72
7.72	22	1 0 1	11.46
7.46	17	0 1 1	11.86
7.16	9	0 2 0	12.36
6.79	10	1 1 1	13.02
6.56	8	1 2 0	13.48
5.53	29	0 2 1+	16.00
5.13	4	3 1 0	17.26
4.65	3	3 0 1	19.06
4.59	8	2 2 1+	19.32
4.371	63	0 0 2	20.30
4.223	4	1 0 2	21.02
4.130	3	2 3 0+	21.50
4.052	43	1 1 2+	21.92
3.966	4	4 1 0	22.40
3.864	1	2 0 2	23.00
3.729	13	0 2 2+	23.84
3.639	11	1 2 2	24.44
3.582	1	0 4 0	24.84
3.399	4	2 2 2	26.20
3.329	4	3 1 2	26.76
3.314	3	4 2 1+	26.88
3.123	1	4 3 0	28.56
3.089	2	3 2 2	28.88
2.855	4	0 1 3	31.30
2.840	2	3 4 1+	31.48
2.704	2	4 4 0+	33.10
2.664	1	1 2 3	33.62
2.585	2	4 4 1+	34.68
2.541	1	3 5 0+	35.30
2.535	1	3 1 3	35.38
2.3008	1	5 3 2+	39.12
2.2807	1	1 6 1+	39.48
2.2490	1	7 1 1	40.06
2.1965	1	3 5 2	41.06
2.1642	1	5 5 0+	41.70
2.1244	1	3 6 1+	42.52
2.0907	1	0 2 4+	43.24
2.0742	1	1 2 4	43.60
2.0554	1	7 1 2+	44.02
2.0266	1	2 2 4+	44.68
1.9894	1	8 1 1+	45.56
1.9538	1	3 2 4+	46.44
1.9349	1	2 7 1+	46.92
1.8690	1	4 6 2+	48.68

Δ^9-Tetrahydrocannabinolic Acid B, $C_{22}H_{30}O_4$ - (continued)

Calculated Pattern (Integrated)			
d(Å)	I	hkℓ	2Θ(°) λ - 1.540598Å
10.82	100	1 1 0	8.16
8.26	6	2 0 0	10.71
7.73	22	1 0 1	11.44
7.46	16	0 1 1	11.85
7.16	9	0 2 0	12.35
6.80	10	1 1 1	13.01
6.57	7	1 2 0	13.46
5.54	19	0 2 1	15.98
5.54	11	2 1 1	15.99
5.14	4	3 1 0	17.24
4.66	3	3 0 1	19.04
4.60	6	2 2 1	19.28
4.59	4	1 3 0	19.33
4.430	4	3 1 1	20.03
4.372	69	0 0 2	20.30
4.226	4	1 0 2	21.00
4.134	2	2 3 0	21.48
4.062	16	1 3 1	21.86
4.054	35	1 1 2	21.91
3.967	3	4 1 0	22.39
3.864	1	2 0 2	23.00
3.737	2	2 3 1	23.79
3.732	10	0 2 2	23.83
3.731	3	2 1 2	23.83
3.640	12	1 2 2	24.43
3.613	1	4 1 1	24.62
3.581	1	0 4 0	24.84
3.424	1	3 0 2	26.01
3.401	4	2 2 2	26.18
3.330	4	3 1 2	26.75
3.314	1	0 4 1	26.88
3.311	2	4 2 1	26.91
3.123	2	4 3 0	28.56
3.089	2	3 2 2	28.88
2.856	4	0 1 3	31.29
2.839	2	3 4 1	31.48
2.705	2	4 4 0	33.09
2.700	1	0 2 3	33.16
2.664	1	1 2 3	33.61
2.584	1	4 4 1	34.68
2.535	1	3 1 3	35.38
2.2496	1	7 1 1	40.05
2.1972	1	3 5 2	41.05
2.1643	1	5 5 0	41.70
2.1427	1	1 1 4	42.14
2.1247	1	3 6 1	42.51
2.0742	1	1 2 4	43.60
2.0268	1	2 2 4	44.67
1.9897	1	8 1 1	45.55

Vinbarbital, Form I, $C_{11}H_{16}N_2O_3$

Synonyms
1. 5-Ethyl-5(1-methyl-1-butenyl) barbituric acid

Structure
Monoclinic, $P2_1/c$ (14), Z = 4. The structure was determined by Craven and Cusatis [1969].

Atom positions
All atoms are in general positions 4(e). The reference was lacking data for H(221); it was omitted from these calculations.

Polymorphism
Two polymorphs (melting points 129° and 106°) have been reported but they are very difficult to prepare from melt or solution [Craven and Cusatis, 1969].

Lattice constants
a = 14.396(5) Å
b = 6.822(3)
c = 12.541(7)
β = 107.43(3)°

a/b = 2.1102
c/b = 1.8383

(published values: a = 14.395(5) Å, b = 6.822(3), c = 12.540(7), β = 107° 26(2)' [Craven and Cusatis, 1969]

Volume
1175.1 $Å^3$

Density
(calculated) 1.268 g/cm^3

Thermal parameters
Anisotropic for non-hydrogen atoms [Craven and Cusatis, 1969]. Overall B = 5.0 for hydrogen atoms.

Scattering factors
C^0, H^0, N^0, O^0 [International Tables, 1962]

Scale factors (integrated intensities)
$\gamma = 2.068 \times 10^{-3}$
$I/I_{corundum}$ (calculated) = 0.799 for reflection with hkℓ = 110.

Additional pattern
1. PDF card 9-555 [Parkes, E. B., South Western Forensic Science Lab., Westbury-on-Trym, Bristol, Eng.]

References
Craven, B. M. and Cusatis, C. (1969). Acta Crystallogr. B25, 2291.
International Tables for X-ray Crystallography, III (1962). (The Kynoch Press, Birmingham, Eng.) p. 202.

Calculated Pattern (Peak heights)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
13.71	99	1 0 0	6.44
6.87	10	2 0 0	12.88
6.20	26	-1 0 2	14.28
6.10	100	1 1 0	14.50
5.981	34	0 0 2	14.80
5.925	33	0 1 1	14.94
5.757	4	-1 1 1	15.38
4.962	22	1 0 2	17.86
4.839	38	2 1 0	18.32
4.591	35	-1 1 2	19.32
4.498	4	0 1 2	19.72
4.308	5	-3 0 2	20.60
4.188	17	2 1 1	21.20
4.015	1	1 1 2	22.12
3.914	6	-3 1 1	22.70
3.799	3	3 1 0	23.40
3.645	2	-3 1 2	24.40
3.562	2	-1 1 3	24.98
3.445	20	0 1 3+	25.84
3.388	2	3 1 1	26.28
3.309	3	1 2 0	26.92
3.281	4	0 2 1	27.16
3.202	17	3 0 2	27.84
3.125	19	-1 0 4+	28.54
3.056	9	2 2 0+	29.20
2.988	14	-1 2 2	29.88
2.963	7	0 2 2	30.14
2.897	2	3 1 2	30.84
2.870	11	2 2 1	31.14
2.840	4	-5 0 2+	31.48
2.812	13	1 2 2	31.80
2.746	1	5 0 0	32.58
2.642	6	-1 2 3	33.90
2.592	5	0 2 3+	34.58
2.569	3	3 2 1	34.90
2.472	4	-4 2 1+	36.32
2.464	4	3 1 3	36.44
2.420	3	4 2 0	37.12
2.362	2	5 1 1	38.06
2.335	2	-1 1 5+	38.52
2.295	1	-4 2 3+	39.22
2.253	2	0 1 5+	39.98
2.244	1	1 3 0	40.16
2.227	3	-3 2 4	40.48
2.196	2	-5 2 1	41.06
2.186	1	1 3 1	41.26
2.139	2	5 2 0	42.22
2.063	1	-1 0 6	43.84
2.052	2	-5 1 5+	44.10
2.009	2	-1 2 5+	45.10

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
2.005	2	-4 0 6	45.18
1.972	1	2 3 2+	45.98
1.963	1	7 0 0+	46.22
1.915	2	1 3 3+	47.44
1.898	2	4 2 3+	47.88
1.880	2	5 2 2	48.38
1.854	1	-7 1 4+	49.10
1.782	1	-2 2 6+	51.22
1.722	1	0 2 6+	53.16
1.710	1	-6 2 5	53.56

Calculated Pattern (Integrated)

d(Å)	I	hkℓ	2θ(°) λ - 1.540598Å
13.73	96	1 0 0	6.43
6.87	10	2 0 0	12.88
6.21	19	-1 0 2	14.26
6.11	100	1 1 0	14.49
5.983	26	0 0 2	14.80
5.926	27	0 1 1	14.94
5.761	2	-1 1 1	15.37
4.967	23	1 0 2	17.84
4.840	40	2 1 0	18.32
4.591	37	-1 1 2	19.32
4.498	3	0 1 2	19.72
4.312	5	-3 0 2	20.58
4.224	1	-2 1 2	21.02
4.190	19	2 1 1	21.19
4.016	1	1 1 2	22.12
3.915	7	-3 1 1	22.69
3.802	3	3 1 0	23.38
3.645	2	-3 1 2	24.40
3.564	2	-1 1 3	24.96
3.459	13	-4 0 2	25.74
3.457	4	-2 1 3	25.75
3.443	15	0 1 3	25.86
3.434	1	4 0 0	25.93
3.426	5	2 1 2	25.99
3.388	1	3 1 1	26.28
3.310	3	1 2 0	26.91
3.280	4	0 2 1	27.16
3.202	19	3 0 2	27.84
3.183	1	-4 1 1	28.01
3.174	1	-3 1 3	28.09
3.153	2	1 1 3	28.28
3.133	10	1 2 1	28.47
3.124	15	-1 0 4	28.55
3.067	4	4 1 0	29.09
3.055	8	2 2 0	29.21
2.991	2	0 0 4	29.85
2.989	15	-1 2 2	29.86
2.963	6	0 2 2	30.13
2.940	1	-3 0 4	30.38
2.899	1	3 1 2	30.82
2.870	12	2 2 1	31.14
2.840	1	-1 1 4	31.47
2.840	2	-5 0 2	31.48
2.825	1	-2 1 4	31.64
2.824	1	-4 1 3	31.66
2.812	14	1 2 2	31.80
2.797	5	4 1 1	31.98
2.747	1	5 0 0	32.57
2.655	2	4 0 2	33.74
2.647	1	-5 1 1	33.84
2.643	6	-1 2 3	33.89
2.592	5	0 2 3	34.57
2.585	1	2 2 2	34.68
2.569	3	3 2 1	34.90
2.476	2	-4 2 1	36.26
2.471	2	-3 2 3	36.32
2.463	3	3 1 3	36.45
2.420	3	4 2 0	37.12
2.362	2	5 1 1	38.06
2.336	1	-1 1 5	38.50
2.335	1	3 2 2	38.53
2.258	1	0 1 5	39.89
2.254	1	5 0 2	39.98
2.243	1	1 3 0	40.16
2.227	4	-3 2 4	40.48
2.197	2	-5 2 1	41.06
2.186	1	1 3 1	41.27
2.139	2	5 2 0	42.21
2.063	1	-1 0 6	43.84
2.056	1	-6 1 4	44.01
2.052	2	-5 1 5	44.10
2.009	2	-1 2 5	45.08
2.008	1	2 2 4	45.12
2.005	1	-4 0 6	45.19
1.962	1	7 0 0	46.23
1.916	1	-4 2 5	47.42
1.916	1	1 3 3	47.42
1.914	1	0 1 6	47.46
1.899	2	4 2 3	47.87
1.880	2	5 2 2	48.37
1.854	1	-7 1 4	49.10
1.782	1	-2 2 6	51.22
1.722	1	0 2 6	53.16
1.710	1	-6 2 5	53.55

INORGANIC NAMES

Further work on this program is in progress, and it is anticipated that additional sections will be issued. Therefore, the cumulative index here is not necessarily the concluding index for the project.

m - Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

		Vol. or Sec.	Page
$C_8H_{12}N_2O_3$	Barbital, form IV	15m	130
$C_9H_{14}N_2O_3$	Metharbital	15m	177
$C_{10}H_{12}N_2O_3$	Allobarbital	14m	41
$C_{10}H_{16}ClNO$	(-)-Ephedrine hydrochloride	16m	124
$C_{11}H_{16}N_2O_3$	Vinbarbital, form I	16m	162
$C_{11}H_{18}N_2O_3$	Amobarbital, form I	15m	114
$C_{11}H_{18}N_2O_3$	Amobarbital, form II	15m	117
$C_{12}H_{10}N_2$	Azobenzene	7m	86
$C_{12}H_{12}N_2O_3$	Phenobarbital, form III	16m	144
$C_{12}H_{16}Cl_2CuN_8$	Copper tetrapyrazole chloride	8m	31
$C_{12}H_{16}Cl_2N_8Ni$	Nickel tetrapyrazole chloride	8m	44
$C_{12}H_{16}CuN_{10}O_6$	Copper tetraimidazole nitrate	13m	24
$C_{12}H_{16}N_2$	(N,N)-Dimethyltryptamine	14m	109
$C_{12}H_{16}N_2O$	Bufotenine	15m	133
$C_{12}H_{16}N_2O$	Psilocin	16m	152
$C_{12}H_{22}O_{11}$	Sucrose	11m	66
$C_{12}H_{26}N_2O_4$	Hexamethylenediammonium adipate	7m	121
$C_{13}H_{21}ClN_2O_2$	Procaine hydrochloride	16m	149
$C_{13}H_{21}N_2O_4P$	Psilocybin methanolate	16m	154
$C_{14}H_{11}FO$	4-Acetyl-2'-fluorodiphenyl	8m	91
$C_{14}H_{20}ClN_3S$	Methapyrilene hydrochloride	14m	112
$C_{15}H_{12}O_2$	Dibenzoylmethane	7m	115
$C_{16}H_{13}ClN_2O$	Diazepam	14m	106
$C_{16}H_{13}N$	N-Phenyl-2-naphthylamine	6m	29
$C_{17}H_{19}ClN_2S$	Chlorpromazine	14m	60
$C_{17}H_{20}ClNO_3 \cdot 3H_2O$	Morphine hydrochloride hydrate	16m	133
$C_{17}H_{22}ClNO_4$	L-Cocaine hydrochloride	16m	114
$C_{17}H_{26}ClN$	Phencyclidine hydrochloride	16m	141
$C_{18}H_{22}BrNO_3 \cdot 2H_2O$	Codeine hydrobromide hydrate	16m	117
$C_{18}H_{24}CdN_{14}O_6$	Cadmium hexaimidazole nitrate	8m	23
$C_{18}H_{24}N_{14}NiO_6$	Nickel hexaimidazole nitrate	7m	27
$C_{18}H_{28}N_2O_4S$	(+)-Amphetamine sulfate	15m	119
$C_{19}H_{22}ClNO_4 \cdot 2H_2O$	Naloxone hydrochloride hydrate	16m	136
$C_{19}H_{25}ClN_2$	Imipramine hydrochloride	16m	129
$C_{20}H_{26}ClNO_3$	Benactyzine hydrochloride	16m	92
$C_{20}H_{34}$	α-Dihydrophyllocladene, hartite (or bombiccite)	16m	122
$C_{21}H_{23}ClFNO_2$	Haloperidol	16m	127
$C_{21}H_{30}O_2$	Cannabidiol	16m	111
$C_{22}H_{30}O_4$	Δ^9-Tetrahydrocannabinolic acid B	16m	160
$C_{24}H_{32}N_2O_2Pd$	Palladium bis-(N-isopropyl-3-ethylsalicylaldiminate)	7m	144
$C_{25}H_{15}N_6$	N-Methylphenazinium-7,7,8,8-tetracyanoquinodimethanide	7m	146
$C_{33}H_{40}N_2O_9$	Reserpine	8m	123

		Vol. or Sec.	Page
2-Naphthylamine, N-phenyl-	$C_{10}H_7NHC_6H_5$	6m	29
Neodymium ethylsulfate hydrate	$Nd[(C_2H_5)SO_4]_3 \cdot 9H_2O$	9	41
Nickel acetate hydrate	$Ni(C_2H_3O_2)_2 \cdot 4H_2O$	13m	31
Nickel hexaimidazole nitrate	$Ni(C_3H_4N_2)_6(NO_3)_2$	7m	27
Nickel tetrapyrazole chloride	$Ni(C_3H_4N_2)_4Cl_2$	8m	44
Nicotinic acid	$C_6H_5NO_2$	16m	54
Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (α-HMX)	$C_4H_8N_8O_8$	11m	100
Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (β-HMX)	$C_4H_8N_8O_8$	11m	102
Oxalic acid hydrate	$C_2H_2O_4 \cdot 2H_2O$	16m	55
Palladium bis-(N-isopropyl-3-ethylsalicylaldiminate)	$Pd(C_{12}H_{16}NO)_2$	7m	144
Phencyclidine hydrochloride	$C_{17}H_{26}ClN$	16m	141
Phenobarbital, form III	$C_{12}H_{12}N_2O_3$	16m	144
Picric acid	$C_6H_3N_3O_7$	16m	56
Pimelic acid	$(CH_2)_5(CO_2H)_2$	7m	153
Potassium formate-formic acid complex	$KO_2CH \cdot HO_2CH$	9m	93
Potassium hydrogen o-phthalate	$C_6H_4(COOH)(COOK)$	4m	30
Potassium oxalate hydrate	$K_2C_2O_4 \cdot H_2O$	9m	39
Potassium oxalate perhydrate	$K_2C_2O_4 \cdot H_2O_2$	9m	96
Potassium sodium tartrate hydrate	$C_4H_4KNaO_6 \cdot 4H_2O$	15m	55
Procaine hydrochloride	$C_{13}H_{21}ClN_2O_2$	16m	149
Psilocin	$C_{12}H_{16}N_2O$	16m	152
Psilocybin methanolate	$C_{13}H_{21}N_2O_4P$	16m	154
Reserpine	$C_{33}H_{40}N_2O_9$	8m	123
Rubidium oxalate perhydrate	$Rb_2C_2O_4 \cdot H_2O_2$	9m	102
Silver oxalate	$Ag_2C_2O_4$	9m	47
Sodium acetate hydrate	$C_2H_3NaO_2 \cdot 3H_2O$	15m	66
Sodium barbital	$C_8H_{11}N_2NaO_3$	16m	157
Sodium D-tartrate hydrate	$(CHOH\text{-}CO_2Na)_2 \cdot 2H_2O$	11m	110
Sodium oxalate	$Na_2C_2O_4$	6m	70
Strontium formate	$Sr(CHO_2)_2$	8	55
Strontium formate hydrate	$Sr(CHO_2)_2 \cdot 2H_2O$ (orthorhombic)	8	56
Sucrose	$C_{12}H_{22}O_{11}$	11m	66
Tartaric acid, D-	$(CHOHCO_2H)_2$	7m	168
Δ^9-Tetrahydrocannabinolic acid B	$C_{22}H_{30}O_4$	16m	160
Thallium hydrogen phthalate	$C_8H_5O_4Tl$	16m	75
Trimethylammonium chloride	$(CH_3)_3NHCl$	9m	113
2,4,6-Trinitrophenetole	$C_2H_5OC_6H_2(NO_2)_3$	8m	152
Urea	$CO(NH_2)_2$	7	61
Uric acid, phase 1, (calc. pattern)	$C_5H_4N_4O_3$	8m	154
Uric acid (phase 1)	$C_5H_4N_4O_3$	16m	78
Vinbarbital, form I	$C_{11}H_{16}N_2O_3$	16m	162
Zinc diimidazole chloride	$Zn(C_3H_4N_2)_2Cl_2$	7m	123
Zinc glutamate hydrate	$Zn(O_2CCHNH_2CH_2CH_2CO_2) \cdot 2H_2O$	7m	170

*Natural mineral

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16. ABSTRACT *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)*

Standard x-ray diffraction patterns are presented for 87 substances. Fifty-nine of these patterns represent experimental data and 28 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

17. KEY WORDS *(six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons)* Crystal structure; integrated intensities; lattice constants; peak intensities; powder patterns; reference intensities; standard; x-ray diffraction.

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